



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 05:22 AM UTC

PDB ID : 2JZC / pdb_00002jzc
BMRB ID : 15617
Title : NMR solution structure of ALG13: The sugar donor subunit of a yeast N-acetylglucosamine transferase. Northeast Structural Genomics Consortium target YG1
Authors : Wang, X.; Weldeghorghis, T.; Zhang, G.; Imepriali, B.; Montelione, G.T.; Prestegard, J.H.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-01-04

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

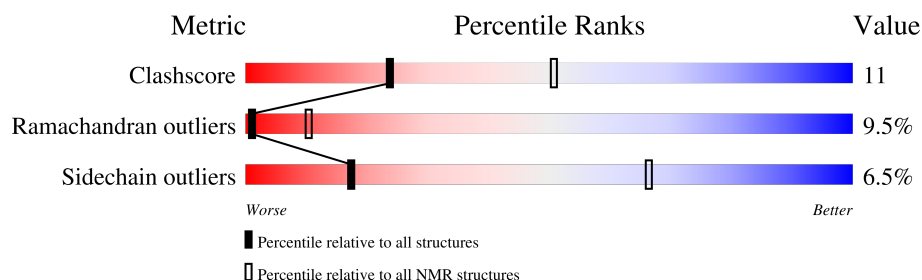
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 54%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	224	

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:27-A:90, A:104-A:209 (170)	1.99	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 4, 5, 6, 7, 8
2	2, 10
Single-model clusters	9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3170 atoms, of which 1586 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UDP-N-acetylglucosamine transferase subunit ALG13.

Mol	Chain	Residues	Atoms						Trace
1	A	201	Total	C	H	N	O	S	0
			3170	1010	1586	266	299	9	

There are 23 discrepancies between the modelled and reference sequences:

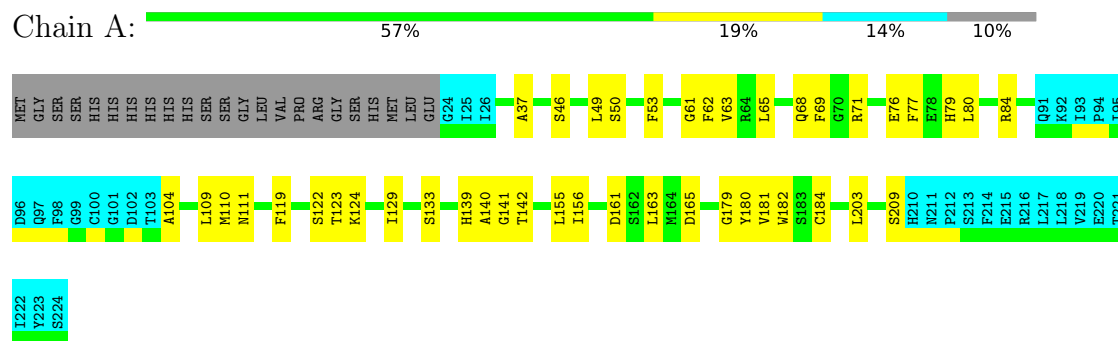
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P53178
A	2	GLY	-	expression tag	UNP P53178
A	3	SER	-	expression tag	UNP P53178
A	4	SER	-	expression tag	UNP P53178
A	5	HIS	-	expression tag	UNP P53178
A	6	HIS	-	expression tag	UNP P53178
A	7	HIS	-	expression tag	UNP P53178
A	8	HIS	-	expression tag	UNP P53178
A	9	HIS	-	expression tag	UNP P53178
A	10	HIS	-	expression tag	UNP P53178
A	11	SER	-	expression tag	UNP P53178
A	12	SER	-	expression tag	UNP P53178
A	13	GLY	-	expression tag	UNP P53178
A	14	LEU	-	expression tag	UNP P53178
A	15	VAL	-	expression tag	UNP P53178
A	16	PRO	-	expression tag	UNP P53178
A	17	ARG	-	expression tag	UNP P53178
A	18	GLY	-	expression tag	UNP P53178
A	19	SER	-	expression tag	UNP P53178
A	20	HIS	-	expression tag	UNP P53178
A	21	MET	-	expression tag	UNP P53178
A	22	LEU	-	expression tag	UNP P53178
A	23	GLU	-	expression tag	UNP P53178

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: UDP-N-acetylglucosamine transferase subunit ALG13

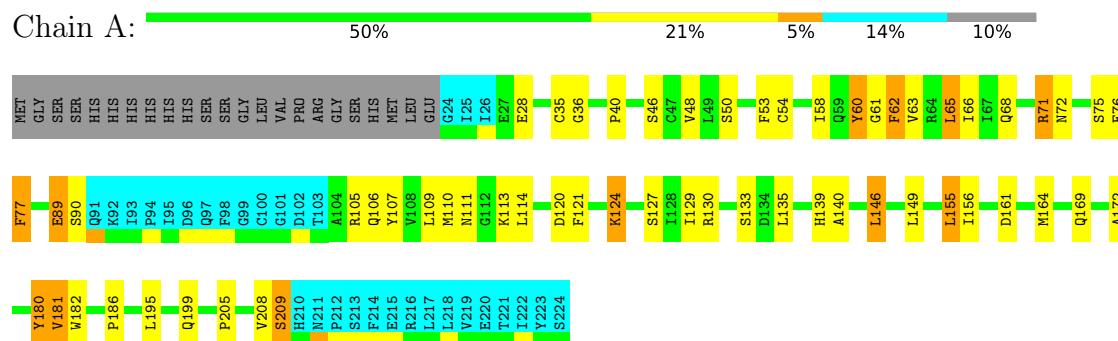


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

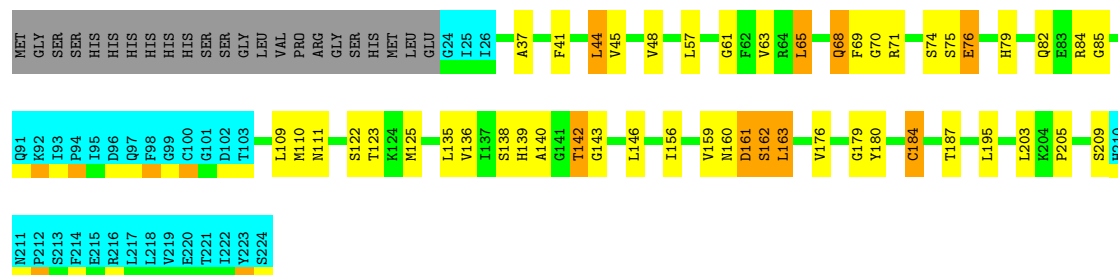
- Molecule 1: UDP-N-acetylglucosamine transferase subunit ALG13



4.2.5 Score per residue for model 5

- Molecule 1: UDP-N-acetylglucosamine transferase subunit ALG13

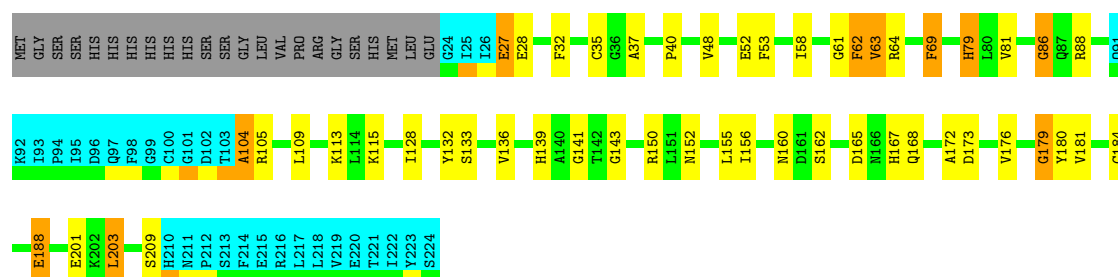
Chain A: 



4.2.6 Score per residue for model 6

- Molecule 1: UDP-N-acetylglucosamine transferase subunit ALG13

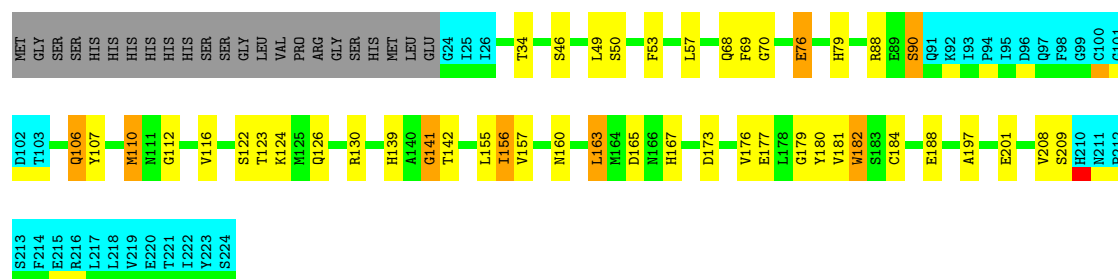
Chain A: 



4.2.7 Score per residue for model 7

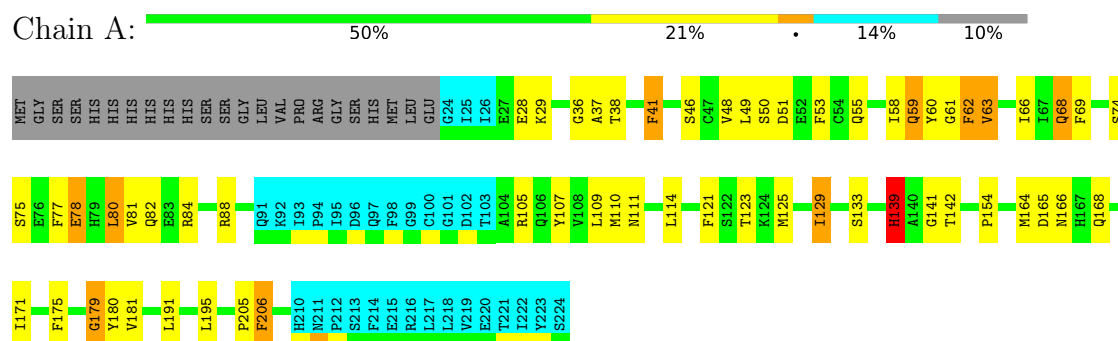
- Molecule 1: UDP-N-acetylglucosamine transferase subunit ALG13

Chain A: 



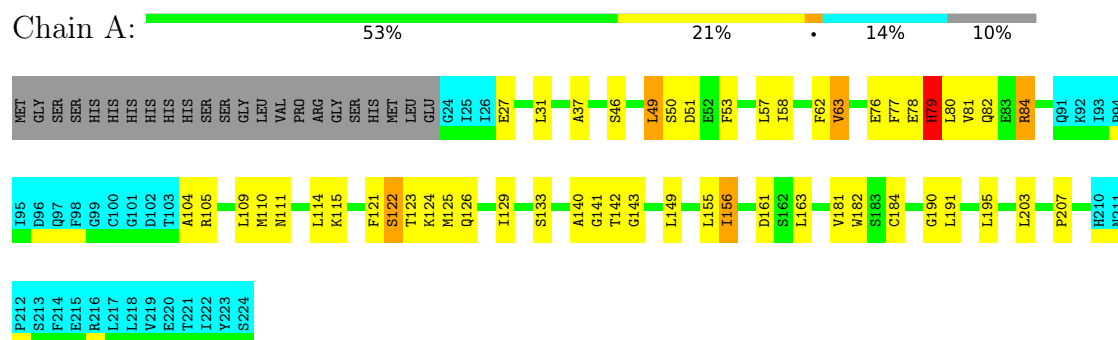
4.2.8 Score per residue for model 8

- Molecule 1: UDP-N-acetylglucosamine transferase subunit ALG13



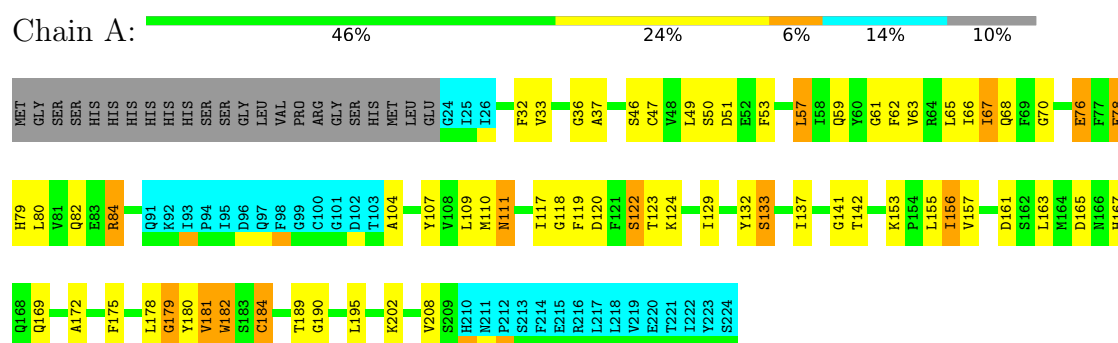
4.2.9 Score per residue for model 9

- Molecule 1: UDP-N-acetylglucosamine transferase subunit ALG13



4.2.10 Score per residue for model 10

- Molecule 1: UDP-N-acetylglucosamine transferase subunit ALG13



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1611
Number of shifts mapped to atoms	1524
Number of unparsed shifts	0
Number of shifts with mapping errors	87
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.89±0.03	0±0/1364 (0.0± 0.0%)	0.93±0.01	0±0/1843 (0.0± 0.0%)
All	All	0.89	0/13640 (0.0%)	0.93	1/18430 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	62	PHE	CA-CB-CG	-5.46	108.34	113.80	3	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1338	1345	1342	29±5
All	All	13380	13450	13420	291

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LEU:C	1:A:156:ILE:HD13	0.70	2.10	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:GLY:O	1:A:62:PHE:O	0.66	2.13	3	4
1:A:173:ASP:O	1:A:176:VAL:HG22	0.66	1.90	6	1
1:A:179:GLY:O	1:A:181:VAL:N	0.64	2.31	6	4
1:A:66:ILE:N	1:A:66:ILE:HD12	0.61	2.10	3	1
1:A:134:ASP:N	1:A:153:LYS:HZ1	0.61	1.92	2	1
1:A:175:PHE:O	1:A:179:GLY:N	0.61	2.33	10	2
1:A:60:TYR:CD1	1:A:195:LEU:HD12	0.61	2.29	8	1
1:A:181:VAL:O	1:A:182:TRP:C	0.61	2.43	10	3
1:A:132:TYR:CD2	1:A:133:SER:N	0.59	2.70	6	2
1:A:46:SER:O	1:A:50:SER:N	0.59	2.36	10	8
1:A:156:ILE:HD12	1:A:156:ILE:N	0.59	2.12	1	1
1:A:155:LEU:HD23	1:A:155:LEU:N	0.59	2.13	6	2
1:A:27:GLU:CD	1:A:115:LYS:HZ2	0.57	2.06	9	1
1:A:65:LEU:C	1:A:65:LEU:HD22	0.57	2.24	5	1
1:A:71:ARG:NE	1:A:71:ARG:N	0.56	2.52	2	1
1:A:180:TYR:O	1:A:203:LEU:HD22	0.56	2.00	2	2
1:A:50:SER:OG	1:A:51:ASP:N	0.55	2.40	8	5
1:A:181:VAL:HG13	1:A:182:TRP:H	0.55	1.62	9	1
1:A:142:THR:N	1:A:168:GLN:HE22	0.54	2.00	3	1
1:A:156:ILE:HD13	1:A:156:ILE:N	0.54	2.17	9	4
1:A:32:PHE:CZ	1:A:66:ILE:HD13	0.54	2.37	10	1
1:A:181:VAL:HG22	1:A:181:VAL:O	0.54	2.02	3	1
1:A:203:LEU:C	1:A:203:LEU:HD22	0.54	2.27	6	1
1:A:132:TYR:CG	1:A:133:SER:N	0.54	2.76	6	2
1:A:65:LEU:C	1:A:66:ILE:HD12	0.54	2.27	10	1
1:A:129:ILE:O	1:A:133:SER:N	0.53	2.41	1	5
1:A:32:PHE:CE1	1:A:132:TYR:CZ	0.53	2.96	6	1
1:A:71:ARG:NH2	1:A:72:ASN:HD21	0.53	2.02	1	1
1:A:176:VAL:HG13	1:A:177:GLU:N	0.53	2.19	7	1
1:A:133:SER:O	1:A:153:LYS:NZ	0.52	2.43	10	1
1:A:71:ARG:NE	1:A:71:ARG:H	0.51	2.04	2	1
1:A:32:PHE:CE2	1:A:68:GLN:NE2	0.51	2.78	3	1
1:A:139:HIS:CD2	1:A:168:GLN:NE2	0.51	2.78	8	1
1:A:181:VAL:O	1:A:182:TRP:CD1	0.51	2.63	9	1
1:A:64:ARG:NH1	1:A:115:LYS:NZ	0.50	2.59	6	1
1:A:67:ILE:HD13	1:A:68:GLN:N	0.50	2.21	10	1
1:A:155:LEU:C	1:A:155:LEU:HD13	0.50	2.31	9	1
1:A:69:PHE:CZ	1:A:77:PHE:CE1	0.50	3.00	2	1
1:A:84:ARG:O	1:A:85:GLY:C	0.50	2.54	2	1
1:A:88:ARG:O	1:A:90:SER:N	0.50	2.44	4	1
1:A:45:VAL:O	1:A:48:VAL:HG22	0.50	2.07	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:ASP:N	1:A:153:LYS:NZ	0.50	2.59	2	1
1:A:61:GLY:C	1:A:62:PHE:CG	0.50	2.89	10	1
1:A:181:VAL:O	1:A:181:VAL:HG13	0.50	2.06	7	1
1:A:185:ALA:O	1:A:187:THR:N	0.49	2.43	4	2
1:A:197:ALA:O	1:A:201:GLU:N	0.49	2.45	7	2
1:A:176:VAL:O	1:A:179:GLY:N	0.49	2.46	5	1
1:A:76:GLU:CD	1:A:76:GLU:N	0.49	2.71	5	3
1:A:184:CYS:SG	1:A:190:GLY:O	0.49	2.71	9	2
1:A:125:MET:SD	1:A:125:MET:N	0.49	2.86	8	1
1:A:125:MET:SD	1:A:126:GLN:NE2	0.49	2.85	2	1
1:A:44:LEU:HD23	1:A:162:SER:OG	0.49	2.07	5	1
1:A:68:GLN:NE2	1:A:125:MET:SD	0.49	2.86	5	2
1:A:60:TYR:CE2	1:A:199:GLN:NE2	0.48	2.81	1	1
1:A:203:LEU:CD1	1:A:203:LEU:N	0.48	2.77	6	1
1:A:188:GLU:CD	1:A:188:GLU:H	0.48	2.15	6	4
1:A:53:PHE:O	1:A:57:LEU:N	0.48	2.42	7	3
1:A:104:ALA:CB	1:A:119:PHE:H	0.48	2.22	3	1
1:A:109:LEU:O	1:A:111:ASN:N	0.48	2.47	9	6
1:A:88:ARG:NH2	1:A:106:GLN:NE2	0.48	2.62	2	1
1:A:121:PHE:CG	1:A:122:SER:N	0.48	2.81	9	2
1:A:32:PHE:CD1	1:A:129:ILE:HG22	0.48	2.44	2	1
1:A:132:TYR:CD1	1:A:133:SER:N	0.48	2.82	4	1
1:A:73:TYR:C	1:A:75:SER:H	0.47	2.17	2	1
1:A:68:GLN:N	1:A:68:GLN:OE1	0.47	2.47	3	1
1:A:155:LEU:O	1:A:182:TRP:CE3	0.47	2.67	3	1
1:A:153:LYS:O	1:A:155:LEU:N	0.47	2.48	2	1
1:A:176:VAL:O	1:A:180:TYR:N	0.47	2.44	7	1
1:A:125:MET:SD	1:A:126:GLN:N	0.47	2.88	9	1
1:A:141:GLY:C	1:A:143:GLY:H	0.47	2.17	6	1
1:A:206:PHE:CD1	1:A:206:PHE:N	0.47	2.81	8	1
1:A:58:ILE:HD12	1:A:58:ILE:N	0.47	2.25	4	3
1:A:180:TYR:O	1:A:181:VAL:C	0.46	2.57	1	1
1:A:135:LEU:N	1:A:135:LEU:HD22	0.46	2.26	4	1
1:A:157:VAL:HG13	1:A:157:VAL:O	0.46	2.10	10	1
1:A:81:VAL:O	1:A:86:GLY:N	0.46	2.48	6	2
1:A:161:ASP:C	1:A:163:LEU:H	0.46	2.18	3	1
1:A:35:CYS:SG	1:A:69:PHE:CE1	0.46	3.08	3	1
1:A:176:VAL:HG23	1:A:177:GLU:N	0.46	2.25	3	1
1:A:160:ASN:CG	1:A:161:ASP:N	0.46	2.73	3	1
1:A:165:ASP:C	1:A:167:HIS:H	0.46	2.19	3	2
1:A:47:CYS:O	1:A:53:PHE:CD1	0.46	2.69	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:LEU:C	1:A:165:ASP:H	0.46	2.18	2	1
1:A:32:PHE:CD1	1:A:132:TYR:OH	0.45	2.62	6	1
1:A:36:GLY:N	1:A:139:HIS:NE2	0.45	2.63	8	1
1:A:48:VAL:O	1:A:53:PHE:CG	0.45	2.69	1	3
1:A:121:PHE:O	1:A:123:THR:N	0.45	2.50	8	1
1:A:128:ILE:HD12	1:A:128:ILE:N	0.45	2.27	6	2
1:A:188:GLU:CD	1:A:188:GLU:N	0.45	2.75	4	2
1:A:64:ARG:HH12	1:A:115:LYS:HZ2	0.45	1.55	6	1
1:A:106:GLN:NE2	1:A:107:TYR:N	0.45	2.64	7	1
1:A:121:PHE:O	1:A:121:PHE:CD2	0.45	2.70	2	1
1:A:162:SER:O	1:A:163:LEU:C	0.45	2.59	5	1
1:A:142:THR:OG1	1:A:143:GLY:N	0.45	2.49	5	1
1:A:203:LEU:N	1:A:203:LEU:HD13	0.45	2.27	6	1
1:A:208:VAL:HG13	1:A:209:SER:N	0.44	2.27	3	2
1:A:66:ILE:N	1:A:66:ILE:CD1	0.44	2.80	3	1
1:A:123:THR:HG22	1:A:124:LYS:N	0.44	2.27	9	1
1:A:59:GLN:N	1:A:59:GLN:CD	0.44	2.76	10	1
1:A:180:TYR:O	1:A:180:TYR:CD2	0.44	2.71	1	1
1:A:155:LEU:N	1:A:155:LEU:CD2	0.44	2.80	6	2
1:A:68:GLN:OE1	1:A:121:PHE:CE2	0.44	2.70	1	1
1:A:184:CYS:SG	1:A:185:ALA:N	0.44	2.90	2	1
1:A:50:SER:OG	1:A:84:ARG:NH2	0.44	2.50	8	1
1:A:51:ASP:N	1:A:84:ARG:NH2	0.44	2.66	4	1
1:A:77:PHE:CD2	1:A:77:PHE:O	0.44	2.71	8	1
1:A:61:GLY:O	1:A:62:PHE:C	0.44	2.60	8	2
1:A:155:LEU:O	1:A:156:ILE:HD13	0.44	2.13	3	1
1:A:173:ASP:O	1:A:176:VAL:HG12	0.44	2.12	7	1
1:A:46:SER:O	1:A:49:LEU:N	0.44	2.51	9	1
1:A:164:MET:C	1:A:166:ASN:H	0.44	2.20	3	1
1:A:51:ASP:OD1	1:A:84:ARG:NE	0.44	2.50	10	1
1:A:70:GLY:O	1:A:72:ASN:N	0.44	2.50	4	1
1:A:138:SER:OG	1:A:139:HIS:N	0.43	2.50	5	1
1:A:181:VAL:HG13	1:A:182:TRP:N	0.43	2.26	9	1
1:A:169:GLN:O	1:A:172:ALA:N	0.43	2.51	10	2
1:A:156:ILE:N	1:A:156:ILE:CD1	0.43	2.81	9	2
1:A:106:GLN:N	1:A:106:GLN:CD	0.43	2.76	2	2
1:A:30:ALA:O	1:A:134:ASP:HB3	0.43	2.13	4	1
1:A:52:GLU:H	1:A:52:GLU:CD	0.43	2.19	6	1
1:A:65:LEU:HD13	1:A:66:ILE:N	0.43	2.28	1	1
1:A:139:HIS:N	1:A:139:HIS:ND1	0.43	2.63	8	1
1:A:39:VAL:O	1:A:40:PRO:O	0.43	2.37	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:HD11	1:A:113:LYS:HZ3	0.43	1.73	6	1
1:A:31:LEU:N	1:A:31:LEU:HD12	0.43	2.27	9	1
1:A:69:PHE:CE1	1:A:105:ARG:NH2	0.43	2.86	6	1
1:A:35:CYS:O	1:A:139:HIS:CE1	0.43	2.72	1	1
1:A:127:SER:OG	1:A:130:ARG:NH2	0.43	2.52	1	1
1:A:35:CYS:SG	1:A:139:HIS:CD2	0.43	3.12	2	1
1:A:121:PHE:O	1:A:122:SER:O	0.43	2.37	2	1
1:A:84:ARG:NE	1:A:84:ARG:O	0.43	2.51	10	1
1:A:105:ARG:NE	1:A:107:TYR:OH	0.43	2.52	1	1
1:A:73:TYR:C	1:A:75:SER:N	0.43	2.77	2	1
1:A:39:VAL:O	1:A:39:VAL:HG23	0.43	2.13	4	1
1:A:139:HIS:CE1	1:A:168:GLN:NE2	0.43	2.87	4	1
1:A:68:GLN:HE21	1:A:125:MET:CE	0.43	2.27	5	1
1:A:171:ILE:O	1:A:175:PHE:N	0.43	2.51	8	1
1:A:80:LEU:N	1:A:80:LEU:HD12	0.42	2.28	9	1
1:A:176:VAL:CG1	1:A:177:GLU:N	0.42	2.82	7	1
1:A:54:CYS:SG	1:A:113:LYS:NZ	0.42	2.91	1	1
1:A:62:PHE:CD2	1:A:63:VAL:N	0.42	2.88	6	1
1:A:29:LYS:O	1:A:63:VAL:HG21	0.42	2.14	8	1
1:A:82:GLN:N	1:A:82:GLN:CD	0.42	2.77	10	1
1:A:89:GLU:CD	1:A:90:SER:H	0.42	2.22	2	1
1:A:160:ASN:CG	1:A:161:ASP:H	0.42	2.22	3	2
1:A:79:HIS:N	1:A:79:HIS:CD2	0.42	2.86	9	1
1:A:135:LEU:N	1:A:135:LEU:CD2	0.42	2.83	4	1
1:A:119:PHE:CE2	1:A:120:ASP:O	0.42	2.72	10	1
1:A:165:ASP:O	1:A:167:HIS:N	0.42	2.53	10	1
1:A:68:GLN:NE2	1:A:120:ASP:O	0.42	2.51	1	1
1:A:112:GLY:C	1:A:115:LYS:NZ	0.42	2.78	3	1
1:A:81:VAL:HG23	1:A:82:GLN:N	0.42	2.29	4	3
1:A:134:ASP:CG	1:A:135:LEU:H	0.42	2.23	4	1
1:A:82:GLN:O	1:A:85:GLY:N	0.42	2.50	5	1
1:A:33:VAL:HA	1:A:137:ILE:O	0.42	2.14	10	1
1:A:69:PHE:CE1	1:A:77:PHE:CZ	0.42	3.07	2	1
1:A:121:PHE:CD2	1:A:122:SER:N	0.42	2.87	3	1
1:A:69:PHE:CZ	1:A:76:GLU:OE2	0.42	2.72	5	1
1:A:59:GLN:N	1:A:59:GLN:OE1	0.42	2.53	8	1
1:A:81:VAL:HG21	1:A:107:TYR:CD2	0.42	2.49	8	1
1:A:44:LEU:HD22	1:A:44:LEU:N	0.42	2.29	3	1
1:A:41:PHE:CE2	1:A:165:ASP:OD1	0.42	2.72	8	1
1:A:189:THR:HG23	1:A:190:GLY:N	0.42	2.30	10	1
1:A:67:ILE:O	1:A:117:ILE:O	0.41	2.38	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:GLY:C	1:A:72:ASN:H	0.41	2.22	3	1
1:A:156:ILE:CG2	1:A:184:CYS:SG	0.41	3.08	6	1
1:A:78:GLU:O	1:A:80:LEU:N	0.41	2.53	8	1
1:A:50:SER:OG	1:A:84:ARG:NH1	0.41	2.53	9	1
1:A:71:ARG:NH2	1:A:72:ASN:ND2	0.41	2.68	1	1
1:A:155:LEU:C	1:A:156:ILE:HD12	0.41	2.40	1	1
1:A:88:ARG:CZ	1:A:106:GLN:HE21	0.41	2.28	2	1
1:A:119:PHE:CD1	1:A:120:ASP:N	0.41	2.88	2	1
1:A:58:ILE:N	1:A:58:ILE:CD1	0.41	2.83	4	1
1:A:80:LEU:O	1:A:80:LEU:HD13	0.41	2.15	4	1
1:A:55:GLN:O	1:A:59:GLN:NE2	0.41	2.52	8	1
1:A:63:VAL:HG13	1:A:64:ARG:N	0.41	2.29	2	1
1:A:69:PHE:O	1:A:69:PHE:CD2	0.41	2.73	2	1
1:A:165:ASP:C	1:A:167:HIS:N	0.41	2.78	3	3
1:A:132:TYR:OH	1:A:135:LEU:C	0.41	2.64	4	1
1:A:78:GLU:C	1:A:80:LEU:H	0.41	2.24	10	1
1:A:48:VAL:O	1:A:53:PHE:CD2	0.41	2.74	1	1
1:A:60:TYR:OH	1:A:195:LEU:O	0.41	2.39	1	1
1:A:104:ALA:H	1:A:105:ARG:NH1	0.41	2.14	2	1
1:A:159:VAL:N	1:A:184:CYS:O	0.41	2.52	5	1
1:A:106:GLN:NE2	1:A:107:TYR:H	0.41	2.14	7	1
1:A:57:LEU:O	1:A:61:GLY:N	0.41	2.54	5	1
1:A:79:HIS:ND1	1:A:79:HIS:C	0.41	2.79	6	1
1:A:150:ARG:C	1:A:152:ASN:H	0.41	2.24	6	1
1:A:60:TYR:CD2	1:A:60:TYR:O	0.41	2.74	2	1
1:A:51:ASP:N	1:A:51:ASP:OD1	0.41	2.54	3	1
1:A:62:PHE:O	1:A:62:PHE:CD2	0.41	2.74	3	1
1:A:109:LEU:HD22	1:A:109:LEU:N	0.41	2.30	4	1
1:A:123:THR:OG1	1:A:124:LYS:N	0.41	2.54	4	1
1:A:139:HIS:O	1:A:168:GLN:NE2	0.41	2.54	4	1
1:A:124:LYS:O	1:A:127:SER:N	0.40	2.54	1	1
1:A:161:ASP:OD1	1:A:161:ASP:N	0.40	2.54	1	2
1:A:128:ILE:N	1:A:128:ILE:CD1	0.40	2.84	6	2
1:A:164:MET:O	1:A:166:ASN:N	0.40	2.53	8	1
1:A:141:GLY:O	1:A:143:GLY:N	0.40	2.51	9	1
1:A:155:LEU:HD13	1:A:156:ILE:N	0.40	2.31	9	1
1:A:60:TYR:CZ	1:A:199:GLN:CD	0.40	2.99	1	1
1:A:46:SER:OG	1:A:47:CYS:N	0.40	2.54	4	1
1:A:177:GLU:C	1:A:179:GLY:H	0.40	2.24	7	1
1:A:76:GLU:O	1:A:77:PHE:O	0.40	2.39	1	1
1:A:77:PHE:O	1:A:79:HIS:ND1	0.40	2.55	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:C	1:A:65:LEU:CD2	0.40	2.95	5	1
1:A:52:GLU:CD	1:A:52:GLU:N	0.40	2.80	6	1
1:A:126:GLN:O	1:A:130:ARG:NE	0.40	2.54	7	1
1:A:180:TYR:CD2	1:A:180:TYR:O	0.40	2.74	10	1
1:A:110:MET:C	1:A:112:GLY:N	0.40	2.79	7	1
1:A:139:HIS:O	1:A:141:GLY:N	0.40	2.53	7	1
1:A:122:SER:OG	1:A:123:THR:N	0.40	2.55	10	1
1:A:146:LEU:HD21	1:A:208:VAL:O	0.40	2.17	1	1
1:A:108:VAL:C	1:A:109:LEU:HD22	0.40	2.42	4	1
1:A:35:CYS:O	1:A:139:HIS:NE2	0.40	2.54	6	1
1:A:168:GLN:O	1:A:172:ALA:N	0.40	2.50	6	1
1:A:46:SER:O	1:A:50:SER:CB	0.40	2.69	8	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/224 (76%)	129±3 (76±2%)	25±2 (15±1%)	16±3 (10±2%)	1	10
All	All	1700/2240 (76%)	1290 (76%)	248 (15%)	162 (10%)	1	10

All 51 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	63	VAL	8
1	A	110	MET	8
1	A	37	ALA	7
1	A	62	PHE	6
1	A	140	ALA	6
1	A	179	GLY	6
1	A	77	PHE	5
1	A	124	LYS	5
1	A	180	TYR	5
1	A	122	SER	5

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Mol	Chain	Res	Type	Models (Total)
1	A	28	GLU	4
1	A	40	PRO	4
1	A	75	SER	4
1	A	182	TRP	4
1	A	162	SER	4
1	A	76	GLU	4
1	A	79	HIS	4
1	A	142	THR	4
1	A	186	PRO	3
1	A	205	PRO	3
1	A	209	SER	3
1	A	119	PHE	3
1	A	133	SER	3
1	A	154	PRO	3
1	A	74	SER	3
1	A	161	ASP	3
1	A	163	LEU	3
1	A	69	PHE	3
1	A	104	ALA	3
1	A	141	GLY	3
1	A	36	GLY	2
1	A	71	ARG	2
1	A	89	GLU	2
1	A	90	SER	2
1	A	181	VAL	2
1	A	160	ASN	2
1	A	118	GLY	2
1	A	139	HIS	2
1	A	38	THR	2
1	A	123	THR	2
1	A	70	GLY	2
1	A	78	GLU	2
1	A	164	MET	1
1	A	85	GLY	1
1	A	111	ASN	1
1	A	200	THR	1
1	A	27	GLU	1
1	A	86	GLY	1
1	A	208	VAL	1
1	A	68	GLN	1
1	A	207	PRO	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	150/198 (76%)	140±2 (93±1%)	10±2 (7±1%)	17 66
All	All	1500/1980 (76%)	1402 (93%)	98 (7%)	17 66

All 57 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	49	LEU	6
1	A	156	ILE	5
1	A	203	LEU	4
1	A	65	LEU	3
1	A	114	LEU	3
1	A	135	LEU	3
1	A	146	LEU	3
1	A	116	VAL	3
1	A	41	PHE	3
1	A	80	LEU	3
1	A	84	ARG	3
1	A	184	CYS	3
1	A	195	LEU	3
1	A	60	TYR	2
1	A	106	GLN	2
1	A	149	LEU	2
1	A	66	ILE	2
1	A	44	LEU	2
1	A	68	GLN	2
1	A	136	VAL	2
1	A	163	LEU	2
1	A	191	LEU	2
1	A	58	ILE	1
1	A	155	LEU	1
1	A	71	ARG	1
1	A	89	GLU	1
1	A	153	LYS	1
1	A	32	PHE	1
1	A	130	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	69	PHE	1
1	A	132	TYR	1
1	A	142	THR	1
1	A	123	THR	1
1	A	187	THR	1
1	A	48	VAL	1
1	A	53	PHE	1
1	A	109	LEU	1
1	A	188	GLU	1
1	A	201	GLU	1
1	A	34	THR	1
1	A	157	VAL	1
1	A	160	ASN	1
1	A	59	GLN	1
1	A	88	ARG	1
1	A	129	ILE	1
1	A	139	HIS	1
1	A	206	PHE	1
1	A	63	VAL	1
1	A	78	GLU	1
1	A	79	HIS	1
1	A	57	LEU	1
1	A	67	ILE	1
1	A	76	GLU	1
1	A	107	TYR	1
1	A	111	ASN	1
1	A	178	LEU	1
1	A	202	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 54% for the well-defined parts and 55% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1611
Number of shifts mapped to atoms	1524
Number of unparsed shifts	0
Number of shifts with mapping errors	87
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 87 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	SER	HB2	3.853	0.05	2
1	A	3	SER	C	174.6	0.5	1
1	A	4	SER	H	8.467	0.05	1
1	A	4	SER	C	174.7	0.5	1
1	A	4	SER	CA	59.3	0.5	1
1	A	4	SER	CB	63.6	0.5	1
1	A	4	SER	N	118.038	0.5	1
1	A	5	HIS	H	8.648	0.05	1
1	A	5	HIS	C	175.2	0.5	1
1	A	5	HIS	CA	55.4	0.5	1
1	A	5	HIS	CB	28.7	0.5	1
1	A	5	HIS	N	123.738	0.5	1
1	A	6	HIS	C	176.9	0.5	1
1	A	12	SER	HA	4.46	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	SER	HB2	3.89	0.05	2
1	A	12	SER	C	174.9	0.5	1
1	A	12	SER	CA	58.7	0.5	1
1	A	12	SER	CB	64.3	0.5	1
1	A	13	GLY	H	8.358	0.05	1
1	A	13	GLY	HA2	3.942	0.05	2
1	A	13	GLY	C	173.8	0.5	1
1	A	13	GLY	CA	45.3	0.5	1
1	A	13	GLY	N	110.338	0.5	1
1	A	14	LEU	H	8.038	0.05	1
1	A	14	LEU	HB2	1.53	0.05	2
1	A	14	LEU	HD11	0.8	0.05	2
1	A	14	LEU	HD12	0.8	0.05	2
1	A	14	LEU	HD13	0.8	0.05	2
1	A	14	LEU	HD21	0.85	0.05	2
1	A	14	LEU	HD22	0.85	0.05	2
1	A	14	LEU	HD23	0.85	0.05	2
1	A	14	LEU	C	177.1	0.5	1
1	A	14	LEU	CA	55.3	0.5	1
1	A	14	LEU	CB	41.7	0.5	1
1	A	14	LEU	CD1	23.4	0.5	1
1	A	14	LEU	CD2	24.8	0.5	1
1	A	14	LEU	CG	27.2	0.5	1
1	A	14	LEU	N	121.438	0.5	1
1	A	15	VAL	H	8.078	0.05	1
1	A	15	VAL	HA	4.35	0.05	1
1	A	15	VAL	HG11	0.86	0.05	2
1	A	15	VAL	HG12	0.86	0.05	2
1	A	15	VAL	HG13	0.86	0.05	2
1	A	15	VAL	HG21	0.88	0.05	2
1	A	15	VAL	HG22	0.88	0.05	2
1	A	15	VAL	HG23	0.88	0.05	2
1	A	15	VAL	CA	59.8	0.5	1
1	A	15	VAL	CB	32.1	0.5	1
1	A	15	VAL	CG1	21.0	0.5	1
1	A	15	VAL	CG2	20.4	0.5	1
1	A	15	VAL	N	122.438	0.5	1
1	A	16	PRO	HA	4.356	0.05	1
1	A	16	PRO	HB2	2.22	0.05	2
1	A	16	PRO	HD2	3.625	0.05	2
1	A	16	PRO	HD3	3.83	0.05	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	PRO	HG2	1.9	0.05	2
1	A	16	PRO	HG3	1.98	0.05	2
1	A	16	PRO	C	176.9	0.5	1
1	A	16	PRO	CA	63.0	0.5	1
1	A	16	PRO	CB	31.8	0.5	1
1	A	17	ARG	H	8.458	0.05	1
1	A	17	ARG	HA	4.26	0.05	1
1	A	17	ARG	HB2	1.81	0.05	2
1	A	17	ARG	HD2	3.16	0.05	2
1	A	17	ARG	HG2	1.64	0.05	2
1	A	17	ARG	C	177.0	0.5	1
1	A	17	ARG	CA	56.4	0.5	1
1	A	17	ARG	CB	30.3	0.5	1
1	A	17	ARG	N	121.738	0.5	1
1	A	18	GLY	H	8.467	0.05	1
1	A	18	GLY	HA2	3.97	0.05	2
1	A	18	GLY	C	174.1	0.5	1
1	A	18	GLY	CA	45.4	0.5	1
1	A	18	GLY	N	110.038	0.5	1
1	A	19	SER	H	8.198	0.05	1
1	A	19	SER	CA	58.8	0.5	1
1	A	19	SER	CB	64.1	0.5	1
1	A	19	SER	N	115.438	0.5	1
1	A	22	LEU	C	175.0	0.5	1
1	A	23	GLU	H	8.288	0.05	1
1	A	23	GLU	HA	4.42	0.05	1
1	A	23	GLU	HB2	2.38	0.05	2
1	A	23	GLU	HB3	2.47	0.05	2
1	A	23	GLU	C	176.4	0.5	1
1	A	23	GLU	CA	55.6	0.5	1
1	A	23	GLU	CB	32.2	0.5	1
1	A	23	GLU	N	120.938	0.5	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	188	-0.42 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	171	0.49 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	183	-0.14 ± 0.09	None needed (< 0.5 ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
^{15}N	185	0.84 ± 0.33	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 54%, i.e. 1274 atoms were assigned a chemical shift out of a possible 2338. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	629/850 (74%)	182/346 (53%)	296/340 (87%)	151/164 (92%)
Sidechain	623/1307 (48%)	386/852 (45%)	235/406 (58%)	2/49 (4%)
Aromatic	22/181 (12%)	21/88 (24%)	0/86 (0%)	1/7 (14%)
Overall	1274/2338 (54%)	589/1286 (46%)	531/832 (64%)	154/220 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 1520 atoms were assigned a chemical shift out of a possible 2761. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	743/1004 (74%)	219/409 (54%)	348/402 (87%)	176/193 (91%)
Sidechain	747/1539 (49%)	463/1003 (46%)	281/480 (59%)	3/56 (5%)
Aromatic	30/218 (14%)	27/106 (25%)	2/103 (2%)	1/9 (11%)
Overall	1520/2761 (55%)	709/1518 (47%)	631/985 (64%)	180/258 (70%)

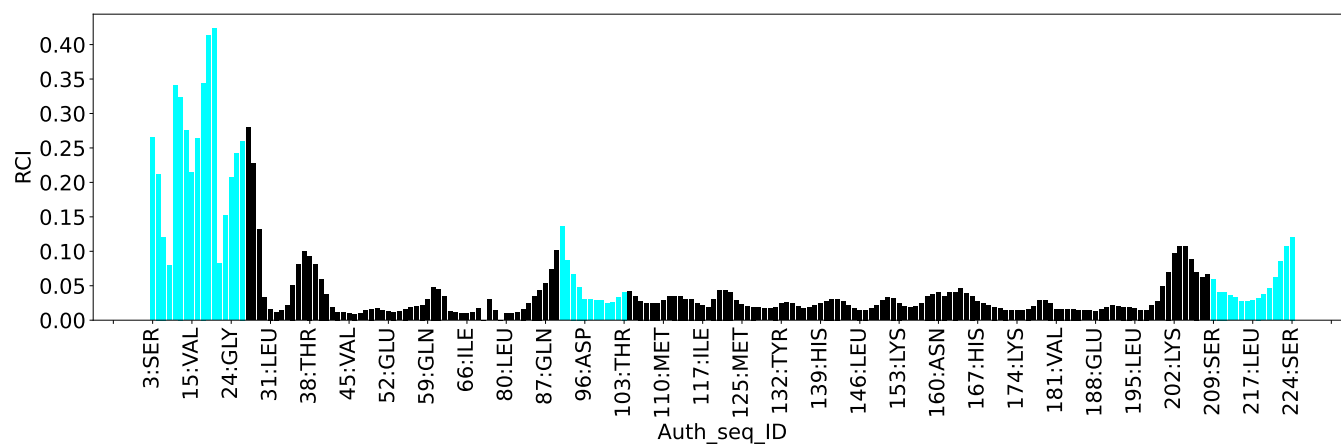
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	901
Intra-residue ($ i-j =0$)	96
Sequential ($ i-j =1$)	223
Medium range ($ i-j >1$ and $ i-j <5$)	251
Long range ($ i-j \geq 5$)	331
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	243
Number of unmapped restraints	0
Number of restraints per residue	5.1
Number of long range restraints per residue ¹	1.5

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	32.2	0.2
0.2-0.5 (Medium)	38.2	0.48
>0.5 (Large)	0.5	1.09

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	37.0	9.69
10.0-20.0 (Medium)	0.2	11.43
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

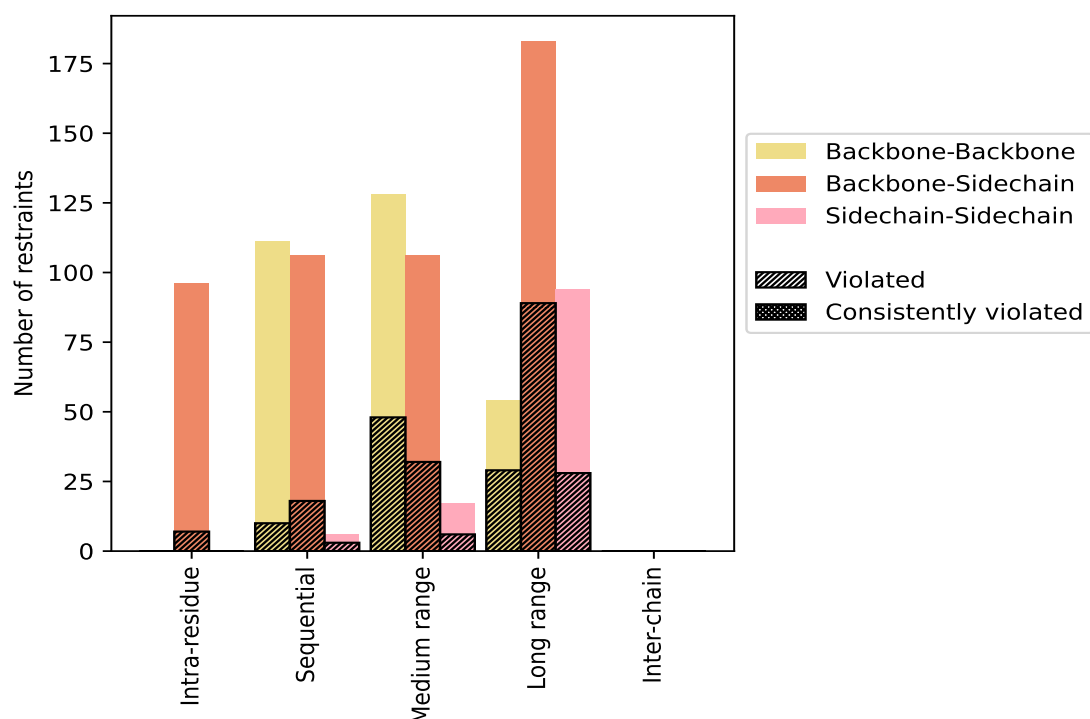
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	96	10.7	7	7.3	0.8	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	96	10.7	7	7.3	0.8	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	223	24.8	31	13.9	3.4	0	0.0	0.0
Backbone-Backbone	111	12.3	10	9.0	1.1	0	0.0	0.0
Backbone-Sidechain	106	11.8	18	17.0	2.0	0	0.0	0.0
Sidechain-Sidechain	6	0.7	3	50.0	0.3	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	251	27.9	86	34.3	9.5	0	0.0	0.0
Backbone-Backbone	128	14.2	48	37.5	5.3	0	0.0	0.0
Backbone-Sidechain	106	11.8	32	30.2	3.6	0	0.0	0.0
Sidechain-Sidechain	17	1.9	6	35.3	0.7	0	0.0	0.0
Long range (i-j ≥5)	331	36.7	146	44.1	16.2	0	0.0	0.0
Backbone-Backbone	54	6.0	29	53.7	3.2	0	0.0	0.0
Backbone-Sidechain	183	20.3	89	48.6	9.9	0	0.0	0.0
Sidechain-Sidechain	94	10.4	28	29.8	3.1	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	901	100.0	270	30.0	30.0	0	0.0	0.0
Backbone-Backbone	293	32.5	87	29.7	9.7	0	0.0	0.0
Backbone-Sidechain	491	54.5	146	29.7	16.2	0	0.0	0.0
Sidechain-Sidechain	117	13.0	37	31.6	4.1	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

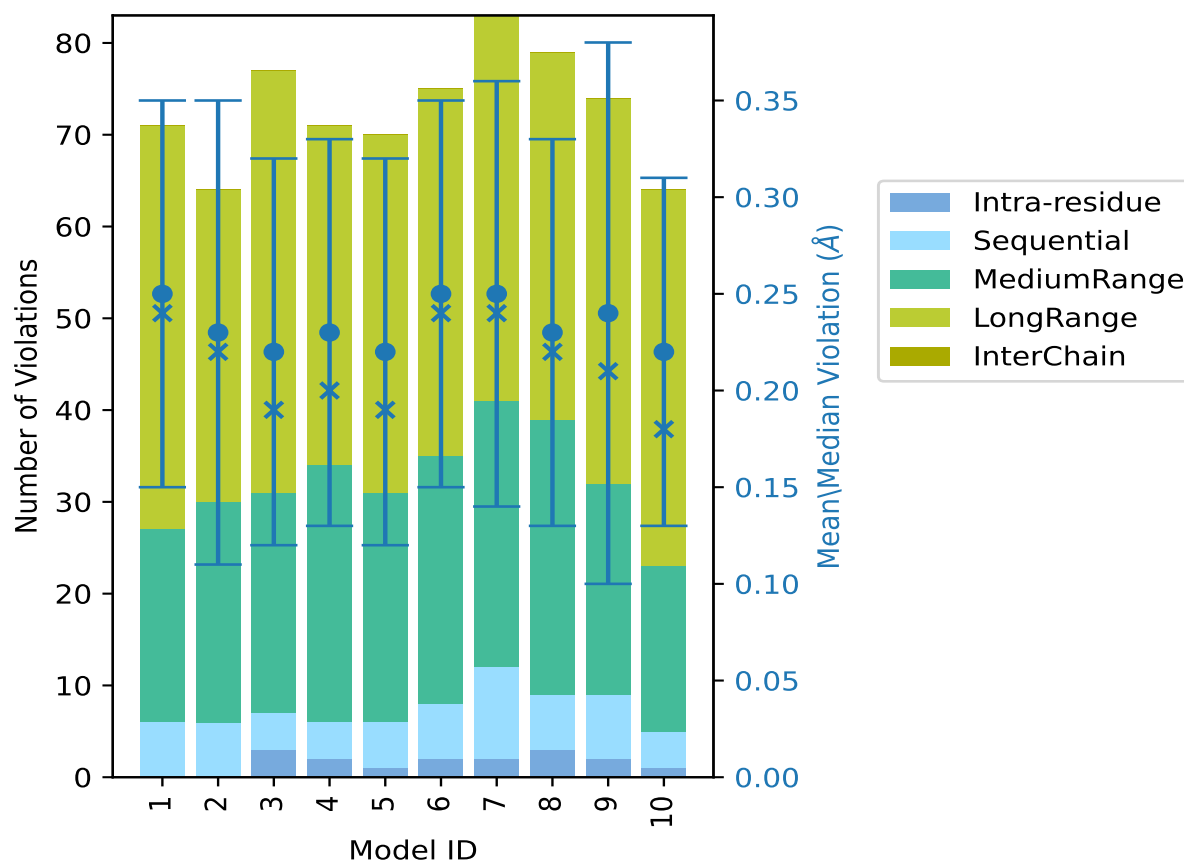
9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	6	21	44	0	71	0.25	0.44	0.1	0.24
2	0	6	24	34	0	64	0.23	0.72	0.12	0.22
3	3	4	24	46	0	77	0.22	0.61	0.1	0.19
4	2	4	28	37	0	71	0.23	0.47	0.1	0.2
5	1	5	25	39	0	70	0.22	0.57	0.1	0.19
6	2	6	27	40	0	75	0.25	0.48	0.1	0.24
7	2	10	29	42	0	83	0.25	0.66	0.11	0.24
8	3	6	30	40	0	79	0.23	0.43	0.1	0.22
9	2	7	23	42	0	74	0.24	1.09	0.14	0.21
10	1	4	18	41	0	64	0.22	0.43	0.09	0.18

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 631(IR:89, SQ:192, MR:165, LR:185, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	19	31	50	0	102	1	10.0
4	5	19	34	0	62	2	20.0
0	3	13	22	0	38	3	30.0

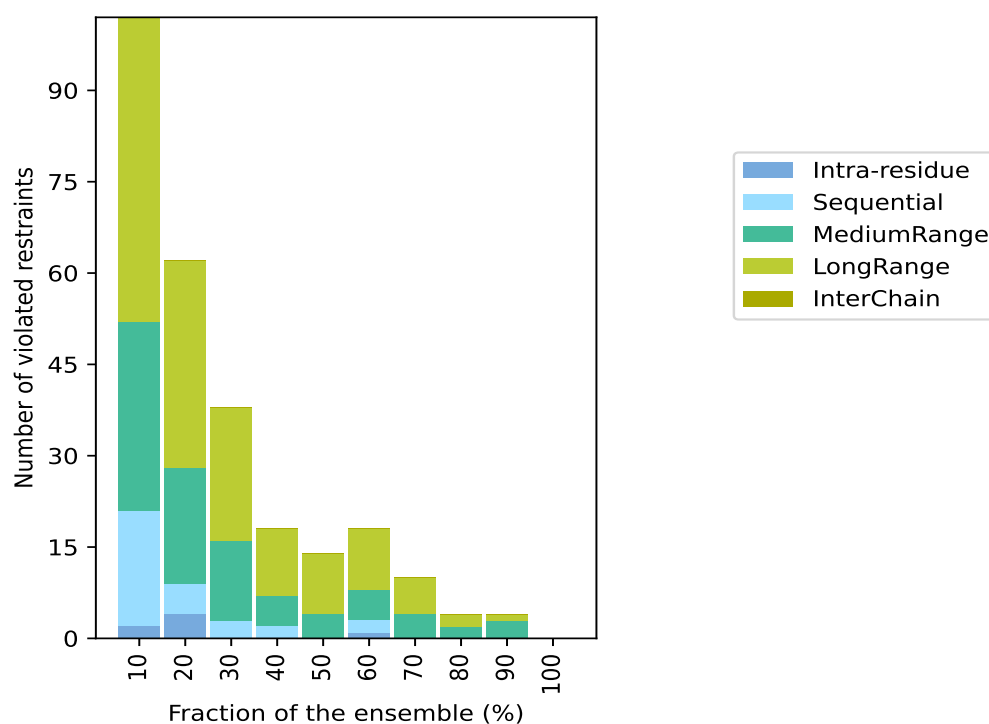
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	2	5	11	0	18	4	40.0
0	0	4	10	0	14	5	50.0
1	2	5	10	0	18	6	60.0
0	0	4	6	0	10	7	70.0
0	0	2	2	0	4	8	80.0
0	0	3	1	0	4	9	90.0
0	0	0	0	0	0	10	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)

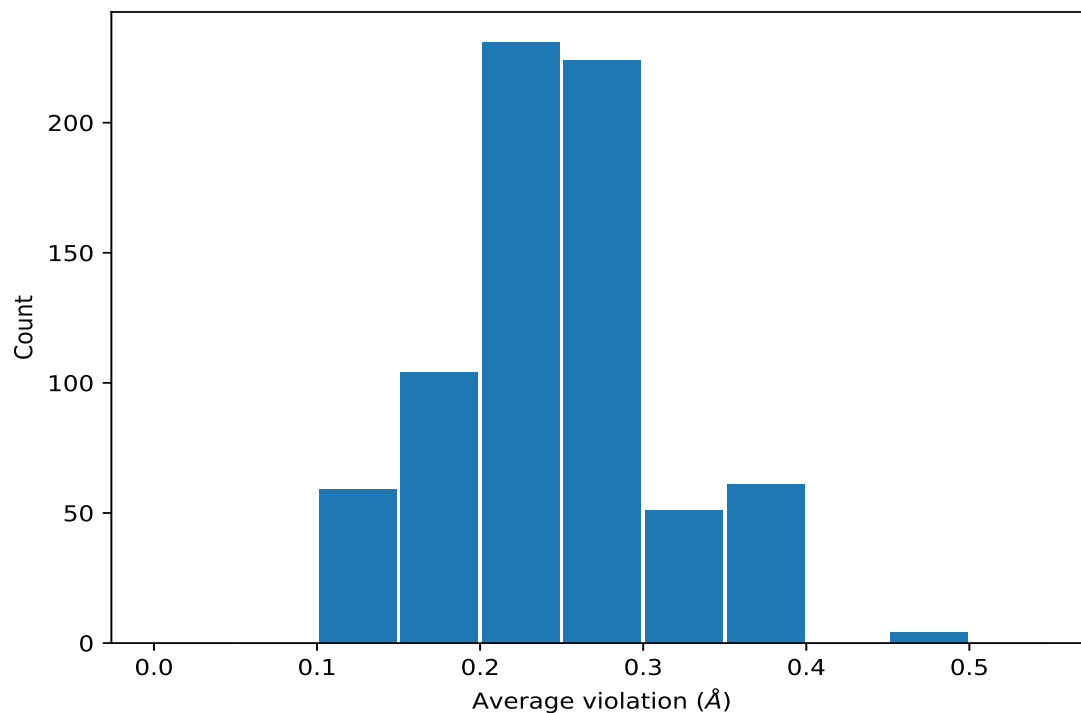


9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	9	0.33	0.07	0.35
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	9	0.29	0.09	0.32
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	9	0.25	0.08	0.24
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	9	0.22	0.09	0.17
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	9	0.22	0.09	0.17
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG21	8	0.3	0.1	0.31
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG22	8	0.3	0.1	0.31
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG23	8	0.3	0.1	0.31
(1,184)	1:49:A:LEU:H	1:51:A:ASP:H	8	0.27	0.08	0.3
(1,168)	1:49:A:LEU:HD11	1:107:A:TYR:H	8	0.22	0.12	0.16
(1,168)	1:49:A:LEU:HD12	1:107:A:TYR:H	8	0.22	0.12	0.16
(1,168)	1:49:A:LEU:HD13	1:107:A:TYR:H	8	0.22	0.12	0.16
(1,457)	1:126:A:GLN:H	1:129:A:ILE:H	8	0.14	0.04	0.11
(1,220)	1:54:A:CYS:H	1:58:A:ILE:H	7	0.34	0.08	0.37
(1,610)	1:150:A:ARG:H	1:153:A:LYS:H	7	0.32	0.07	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG11	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG12	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG13	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG21	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG22	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG23	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG11	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG12	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG13	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG21	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG22	7	0.3	0.12	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG23	7	0.3	0.12	0.3
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD11	7	0.3	0.09	0.29
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD12	7	0.3	0.09	0.29
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD13	7	0.3	0.09	0.29
(1,263)	1:63:A:VAL:H	1:115:A:LYS:H	7	0.24	0.07	0.26
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD11	7	0.22	0.09	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD12	7	0.22	0.09	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD13	7	0.22	0.09	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD21	7	0.22	0.09	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD22	7	0.22	0.09	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD23	7	0.22	0.09	0.2
(1,153)	1:47:A:CYS:H	1:52:A:GLU:H	7	0.19	0.09	0.14
(1,225)	1:55:A:GLN:H	1:58:A:ILE:H	7	0.18	0.02	0.18
(1,46)	1:31:A:LEU:H	1:65:A:LEU:H	7	0.17	0.05	0.16
(1,890)	1:218:A:LEU:H	1:220:A:GLU:H	7	0.15	0.03	0.15
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG11	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG12	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG13	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG21	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG22	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG23	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG11	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG12	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG13	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG21	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG22	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG23	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG11	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG12	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG13	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG21	6	0.36	0.05	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG22	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG23	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG11	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG12	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG13	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG21	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG22	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG23	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG11	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG12	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG13	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG21	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG22	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG23	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG11	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG12	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG13	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG21	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG22	6	0.36	0.05	0.36
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG23	6	0.36	0.05	0.36
(1,359)	1:89:A:GLU:H	1:107:A:TYR:H	6	0.32	0.09	0.32
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG11	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG12	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG13	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG21	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG22	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG23	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG11	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG12	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG13	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG21	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG22	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG23	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG11	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG12	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG13	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG21	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG22	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG23	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG11	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG12	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG13	6	0.3	0.12	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG21	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG22	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG23	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG11	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG12	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG13	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG21	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG22	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG23	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG11	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG12	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG13	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG21	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG22	6	0.3	0.12	0.26
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG23	6	0.3	0.12	0.26
(1,638)	1:156:A:ILE:HD11	1:201:A:GLU:H	6	0.3	0.09	0.34
(1,638)	1:156:A:ILE:HD12	1:201:A:GLU:H	6	0.3	0.09	0.34
(1,638)	1:156:A:ILE:HD13	1:201:A:GLU:H	6	0.3	0.09	0.34
(1,271)	1:64:A:ARG:H	1:115:A:LYS:H	6	0.28	0.07	0.29
(1,506)	1:136:A:VAL:H	1:148:A:SER:H	6	0.27	0.09	0.25
(1,4)	1:25:A:ILE:HD11	1:27:A:GLU:H	6	0.27	0.11	0.29
(1,4)	1:25:A:ILE:HD12	1:27:A:GLU:H	6	0.27	0.11	0.29
(1,4)	1:25:A:ILE:HD13	1:27:A:GLU:H	6	0.27	0.11	0.29
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG21	6	0.27	0.09	0.26
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG22	6	0.27	0.09	0.26
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG23	6	0.27	0.09	0.26
(1,761)	1:181:A:VAL:H	1:183:A:SER:H	6	0.26	0.12	0.22
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG11	6	0.26	0.05	0.25
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG12	6	0.26	0.05	0.25
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG13	6	0.26	0.05	0.25
(1,241)	1:57:A:LEU:HD11	1:59:A:GLN:H	6	0.26	0.08	0.29
(1,241)	1:57:A:LEU:HD12	1:59:A:GLN:H	6	0.26	0.08	0.29
(1,241)	1:57:A:LEU:HD13	1:59:A:GLN:H	6	0.26	0.08	0.29
(1,241)	1:57:A:LEU:HD21	1:59:A:GLN:H	6	0.26	0.08	0.29
(1,241)	1:57:A:LEU:HD22	1:59:A:GLN:H	6	0.26	0.08	0.29
(1,241)	1:57:A:LEU:HD23	1:59:A:GLN:H	6	0.26	0.08	0.29
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD11	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD12	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD13	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD21	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD22	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD23	6	0.25	0.06	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD11	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD12	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD13	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD21	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD22	6	0.25	0.06	0.28
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD23	6	0.25	0.06	0.28
(1,741)	1:178:A:LEU:HD11	1:180:A:TYR:H	6	0.25	0.1	0.26
(1,741)	1:178:A:LEU:HD12	1:180:A:TYR:H	6	0.25	0.1	0.26
(1,741)	1:178:A:LEU:HD13	1:180:A:TYR:H	6	0.25	0.1	0.26
(1,741)	1:178:A:LEU:HD21	1:180:A:TYR:H	6	0.25	0.1	0.26
(1,741)	1:178:A:LEU:HD22	1:180:A:TYR:H	6	0.25	0.1	0.26
(1,741)	1:178:A:LEU:HD23	1:180:A:TYR:H	6	0.25	0.1	0.26
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD11	6	0.25	0.11	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD12	6	0.25	0.11	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD13	6	0.25	0.11	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD21	6	0.25	0.11	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD22	6	0.25	0.11	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD23	6	0.25	0.11	0.27
(1,164)	1:48:A:VAL:HG11	1:53:A:PHE:H	6	0.22	0.08	0.24
(1,164)	1:48:A:VAL:HG12	1:53:A:PHE:H	6	0.22	0.08	0.24
(1,164)	1:48:A:VAL:HG13	1:53:A:PHE:H	6	0.22	0.08	0.24
(1,164)	1:48:A:VAL:HG21	1:53:A:PHE:H	6	0.22	0.08	0.24
(1,164)	1:48:A:VAL:HG22	1:53:A:PHE:H	6	0.22	0.08	0.24
(1,164)	1:48:A:VAL:HG23	1:53:A:PHE:H	6	0.22	0.08	0.24
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG11	6	0.21	0.03	0.22
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG12	6	0.21	0.03	0.22
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG13	6	0.21	0.03	0.22
(1,765)	1:182:A:TRP:HE1	1:197:A:ALA:H	6	0.18	0.04	0.17
(1,185)	1:49:A:LEU:H	1:52:A:GLU:H	6	0.12	0.01	0.12
(1,27)	1:30:A:ALA:H	1:63:A:VAL:H	5	0.45	0.34	0.37
(1,724)	1:176:A:VAL:H	1:180:A:TYR:H	5	0.36	0.08	0.38
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD11	5	0.33	0.08	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD12	5	0.33	0.08	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD13	5	0.33	0.08	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD21	5	0.33	0.08	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD22	5	0.33	0.08	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD23	5	0.33	0.08	0.35
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD11	5	0.31	0.1	0.36
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD12	5	0.31	0.1	0.36
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD13	5	0.31	0.1	0.36
(1,193)	1:49:A:LEU:HD11	1:80:A:LEU:H	5	0.27	0.12	0.21
(1,193)	1:49:A:LEU:HD12	1:80:A:LEU:H	5	0.27	0.12	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,193)	1:49:A:LEU:HD13	1:80:A:LEU:H	5	0.27	0.12	0.21
(1,193)	1:49:A:LEU:HD21	1:80:A:LEU:H	5	0.27	0.12	0.21
(1,193)	1:49:A:LEU:HD22	1:80:A:LEU:H	5	0.27	0.12	0.21
(1,193)	1:49:A:LEU:HD23	1:80:A:LEU:H	5	0.27	0.12	0.21
(1,80)	1:33:A:VAL:H	1:68:A:GLN:H	5	0.26	0.08	0.28
(1,180)	1:49:A:LEU:HD11	1:118:A:GLY:H	5	0.26	0.11	0.29
(1,180)	1:49:A:LEU:HD12	1:118:A:GLY:H	5	0.26	0.11	0.29
(1,180)	1:49:A:LEU:HD13	1:118:A:GLY:H	5	0.26	0.11	0.29
(1,180)	1:49:A:LEU:HD21	1:118:A:GLY:H	5	0.26	0.11	0.29
(1,180)	1:49:A:LEU:HD22	1:118:A:GLY:H	5	0.26	0.11	0.29
(1,180)	1:49:A:LEU:HD23	1:118:A:GLY:H	5	0.26	0.11	0.29
(1,52)	1:32:A:PHE:H	1:135:A:LEU:H	5	0.24	0.09	0.22
(1,567)	1:145:A:ILE:HD11	1:171:A:ILE:H	5	0.22	0.11	0.19
(1,567)	1:145:A:ILE:HD12	1:171:A:ILE:H	5	0.22	0.11	0.19
(1,567)	1:145:A:ILE:HD13	1:171:A:ILE:H	5	0.22	0.11	0.19
(1,568)	1:145:A:ILE:HD11	1:172:A:ALA:H	5	0.22	0.06	0.25
(1,568)	1:145:A:ILE:HD12	1:172:A:ALA:H	5	0.22	0.06	0.25
(1,568)	1:145:A:ILE:HD13	1:172:A:ALA:H	5	0.22	0.06	0.25
(1,262)	1:63:A:VAL:HG11	1:115:A:LYS:H	5	0.21	0.06	0.24
(1,262)	1:63:A:VAL:HG12	1:115:A:LYS:H	5	0.21	0.06	0.24
(1,262)	1:63:A:VAL:HG13	1:115:A:LYS:H	5	0.21	0.06	0.24
(1,262)	1:63:A:VAL:HG21	1:115:A:LYS:H	5	0.21	0.06	0.24
(1,262)	1:63:A:VAL:HG22	1:115:A:LYS:H	5	0.21	0.06	0.24
(1,262)	1:63:A:VAL:HG23	1:115:A:LYS:H	5	0.21	0.06	0.24
(1,29)	1:31:A:LEU:HD11	1:134:A:ASP:H	5	0.18	0.06	0.16
(1,29)	1:31:A:LEU:HD12	1:134:A:ASP:H	5	0.18	0.06	0.16
(1,29)	1:31:A:LEU:HD13	1:134:A:ASP:H	5	0.18	0.06	0.16
(1,29)	1:31:A:LEU:HD21	1:134:A:ASP:H	5	0.18	0.06	0.16
(1,29)	1:31:A:LEU:HD22	1:134:A:ASP:H	5	0.18	0.06	0.16
(1,29)	1:31:A:LEU:HD23	1:134:A:ASP:H	5	0.18	0.06	0.16
(1,204)	1:51:A:ASP:H	1:54:A:CYS:H	5	0.17	0.04	0.16
(1,257)	1:60:A:TYR:H	1:62:A:PHE:H	5	0.14	0.02	0.13
(1,867)	1:203:A:LEU:HD11	1:208:A:VAL:H	4	0.34	0.06	0.35
(1,867)	1:203:A:LEU:HD12	1:208:A:VAL:H	4	0.34	0.06	0.35
(1,867)	1:203:A:LEU:HD13	1:208:A:VAL:H	4	0.34	0.06	0.35
(1,867)	1:203:A:LEU:HD21	1:208:A:VAL:H	4	0.34	0.06	0.35
(1,867)	1:203:A:LEU:HD22	1:208:A:VAL:H	4	0.34	0.06	0.35
(1,867)	1:203:A:LEU:HD23	1:208:A:VAL:H	4	0.34	0.06	0.35
(1,132)	1:44:A:LEU:HD21	1:47:A:CYS:H	4	0.29	0.06	0.29
(1,132)	1:44:A:LEU:HD22	1:47:A:CYS:H	4	0.29	0.06	0.29
(1,132)	1:44:A:LEU:HD23	1:47:A:CYS:H	4	0.29	0.06	0.29
(1,444)	1:116:A:VAL:H	1:118:A:GLY:H	4	0.28	0.07	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,337)	1:81:A:VAL:HG11	1:89:A:GLU:H	4	0.28	0.14	0.27
(1,337)	1:81:A:VAL:HG12	1:89:A:GLU:H	4	0.28	0.14	0.27
(1,337)	1:81:A:VAL:HG13	1:89:A:GLU:H	4	0.28	0.14	0.27
(1,337)	1:81:A:VAL:HG21	1:89:A:GLU:H	4	0.28	0.14	0.27
(1,337)	1:81:A:VAL:HG22	1:89:A:GLU:H	4	0.28	0.14	0.27
(1,337)	1:81:A:VAL:HG23	1:89:A:GLU:H	4	0.28	0.14	0.27
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD11	4	0.27	0.15	0.27
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD12	4	0.27	0.15	0.27
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD13	4	0.27	0.15	0.27
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD11	4	0.27	0.15	0.27
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD12	4	0.27	0.15	0.27
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD13	4	0.27	0.15	0.27
(1,83)	1:34:A:THR:H	1:137:A:ILE:H	4	0.25	0.07	0.24
(1,169)	1:49:A:LEU:HD21	1:107:A:TYR:H	4	0.24	0.12	0.23
(1,169)	1:49:A:LEU:HD22	1:107:A:TYR:H	4	0.24	0.12	0.23
(1,169)	1:49:A:LEU:HD23	1:107:A:TYR:H	4	0.24	0.12	0.23
(1,380)	1:104:A:ALA:H	1:118:A:GLY:H	4	0.23	0.09	0.22
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD11	4	0.22	0.04	0.22
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD12	4	0.22	0.04	0.22
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD13	4	0.22	0.04	0.22
(1,346)	1:84:A:ARG:H	1:86:A:GLY:H	4	0.22	0.04	0.22
(1,495)	1:135:A:LEU:HD11	1:153:A:LYS:H	4	0.22	0.12	0.17
(1,495)	1:135:A:LEU:HD12	1:153:A:LYS:H	4	0.22	0.12	0.17
(1,495)	1:135:A:LEU:HD13	1:153:A:LYS:H	4	0.22	0.12	0.17
(1,495)	1:135:A:LEU:HD21	1:153:A:LYS:H	4	0.22	0.12	0.17
(1,495)	1:135:A:LEU:HD22	1:153:A:LYS:H	4	0.22	0.12	0.17
(1,495)	1:135:A:LEU:HD23	1:153:A:LYS:H	4	0.22	0.12	0.17
(1,1)	1:25:A:ILE:HD11	1:26:A:ILE:H	4	0.2	0.14	0.14
(1,1)	1:25:A:ILE:HD12	1:26:A:ILE:H	4	0.2	0.14	0.14
(1,1)	1:25:A:ILE:HD13	1:26:A:ILE:H	4	0.2	0.14	0.14
(1,670)	1:159:A:VAL:HG11	1:181:A:VAL:H	4	0.2	0.06	0.2
(1,670)	1:159:A:VAL:HG12	1:181:A:VAL:H	4	0.2	0.06	0.2
(1,670)	1:159:A:VAL:HG13	1:181:A:VAL:H	4	0.2	0.06	0.2
(1,670)	1:159:A:VAL:HG21	1:181:A:VAL:H	4	0.2	0.06	0.2
(1,670)	1:159:A:VAL:HG22	1:181:A:VAL:H	4	0.2	0.06	0.2
(1,670)	1:159:A:VAL:HG23	1:181:A:VAL:H	4	0.2	0.06	0.2
(1,794)	1:187:A:THR:H	1:189:A:THR:H	4	0.19	0.06	0.17
(1,671)	1:159:A:VAL:HB	1:183:A:SER:H	4	0.19	0.06	0.19
(1,23)	1:30:A:ALA:H	1:135:A:LEU:H	4	0.17	0.04	0.16
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE1	4	0.16	0.05	0.14
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE2	4	0.16	0.05	0.14
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE1	4	0.16	0.05	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE2	4	0.16	0.05	0.14
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE1	4	0.16	0.05	0.14
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE2	4	0.16	0.05	0.14
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD11	4	0.13	0.02	0.13
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD12	4	0.13	0.02	0.13
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD13	4	0.13	0.02	0.13
(1,410)	1:108:A:VAL:HG11	1:114:A:LEU:H	3	0.38	0.11	0.44
(1,410)	1:108:A:VAL:HG12	1:114:A:LEU:H	3	0.38	0.11	0.44
(1,410)	1:108:A:VAL:HG13	1:114:A:LEU:H	3	0.38	0.11	0.44
(1,410)	1:108:A:VAL:HG21	1:114:A:LEU:H	3	0.38	0.11	0.44
(1,410)	1:108:A:VAL:HG22	1:114:A:LEU:H	3	0.38	0.11	0.44
(1,410)	1:108:A:VAL:HG23	1:114:A:LEU:H	3	0.38	0.11	0.44
(1,110)	1:39:A:VAL:HG21	1:98:A:PHE:HE1	3	0.36	0.15	0.3
(1,110)	1:39:A:VAL:HG21	1:98:A:PHE:HE2	3	0.36	0.15	0.3
(1,110)	1:39:A:VAL:HG22	1:98:A:PHE:HE1	3	0.36	0.15	0.3
(1,110)	1:39:A:VAL:HG22	1:98:A:PHE:HE2	3	0.36	0.15	0.3
(1,110)	1:39:A:VAL:HG23	1:98:A:PHE:HE1	3	0.36	0.15	0.3
(1,110)	1:39:A:VAL:HG23	1:98:A:PHE:HE2	3	0.36	0.15	0.3
(1,487)	1:134:A:ASP:H	1:136:A:VAL:H	3	0.3	0.11	0.3
(1,596)	1:149:A:LEU:HD11	1:153:A:LYS:H	3	0.28	0.04	0.28
(1,596)	1:149:A:LEU:HD12	1:153:A:LYS:H	3	0.28	0.04	0.28
(1,596)	1:149:A:LEU:HD13	1:153:A:LYS:H	3	0.28	0.04	0.28
(1,596)	1:149:A:LEU:HD21	1:153:A:LYS:H	3	0.28	0.04	0.28
(1,596)	1:149:A:LEU:HD22	1:153:A:LYS:H	3	0.28	0.04	0.28
(1,596)	1:149:A:LEU:HD23	1:153:A:LYS:H	3	0.28	0.04	0.28
(1,635)	1:156:A:ILE:HG21	1:198:A:SER:H	3	0.28	0.11	0.29
(1,635)	1:156:A:ILE:HG22	1:198:A:SER:H	3	0.28	0.11	0.29
(1,635)	1:156:A:ILE:HG23	1:198:A:SER:H	3	0.28	0.11	0.29
(1,101)	1:39:A:VAL:HG11	1:44:A:LEU:H	3	0.27	0.15	0.24
(1,101)	1:39:A:VAL:HG12	1:44:A:LEU:H	3	0.27	0.15	0.24
(1,101)	1:39:A:VAL:HG13	1:44:A:LEU:H	3	0.27	0.15	0.24
(1,101)	1:39:A:VAL:HG21	1:44:A:LEU:H	3	0.27	0.15	0.24
(1,101)	1:39:A:VAL:HG22	1:44:A:LEU:H	3	0.27	0.15	0.24
(1,101)	1:39:A:VAL:HG23	1:44:A:LEU:H	3	0.27	0.15	0.24
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD11	3	0.27	0.1	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD12	3	0.27	0.1	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD13	3	0.27	0.1	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD21	3	0.27	0.1	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD22	3	0.27	0.1	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD23	3	0.27	0.1	0.21
(1,310)	1:81:A:VAL:HG11	1:106:A:GLN:H	3	0.27	0.12	0.29
(1,310)	1:81:A:VAL:HG12	1:106:A:GLN:H	3	0.27	0.12	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,310)	1:81:A:VAL:HG13	1:106:A:GLN:H	3	0.27	0.12	0.29
(1,310)	1:81:A:VAL:HG21	1:106:A:GLN:H	3	0.27	0.12	0.29
(1,310)	1:81:A:VAL:HG22	1:106:A:GLN:H	3	0.27	0.12	0.29
(1,310)	1:81:A:VAL:HG23	1:106:A:GLN:H	3	0.27	0.12	0.29
(1,39)	1:31:A:LEU:HD21	1:53:A:PHE:HD1	3	0.26	0.02	0.26
(1,39)	1:31:A:LEU:HD21	1:53:A:PHE:HD2	3	0.26	0.02	0.26
(1,39)	1:31:A:LEU:HD22	1:53:A:PHE:HD1	3	0.26	0.02	0.26
(1,39)	1:31:A:LEU:HD22	1:53:A:PHE:HD2	3	0.26	0.02	0.26
(1,39)	1:31:A:LEU:HD23	1:53:A:PHE:HD1	3	0.26	0.02	0.26
(1,39)	1:31:A:LEU:HD23	1:53:A:PHE:HD2	3	0.26	0.02	0.26
(1,645)	1:157:A:VAL:H	1:159:A:VAL:HB	3	0.26	0.11	0.2
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG11	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG12	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG13	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG21	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG22	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG23	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG11	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG12	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG13	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG21	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG22	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG23	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG11	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG12	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG13	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG21	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG22	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG23	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG11	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG12	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG13	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG21	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG22	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG23	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG11	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG12	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG13	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG21	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG22	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG23	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG11	3	0.24	0.16	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG12	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG13	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG21	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG22	3	0.24	0.16	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG23	3	0.24	0.16	0.15
(1,743)	1:178:A:LEU:H	1:181:A:VAL:H	3	0.24	0.12	0.18
(1,409)	1:108:A:VAL:HG11	1:113:A:LYS:H	3	0.24	0.11	0.25
(1,409)	1:108:A:VAL:HG12	1:113:A:LYS:H	3	0.24	0.11	0.25
(1,409)	1:108:A:VAL:HG13	1:113:A:LYS:H	3	0.24	0.11	0.25
(1,409)	1:108:A:VAL:HG21	1:113:A:LYS:H	3	0.24	0.11	0.25
(1,409)	1:108:A:VAL:HG22	1:113:A:LYS:H	3	0.24	0.11	0.25
(1,409)	1:108:A:VAL:HG23	1:113:A:LYS:H	3	0.24	0.11	0.25
(1,190)	1:49:A:LEU:HD11	1:77:A:PHE:HD1	3	0.23	0.07	0.22
(1,190)	1:49:A:LEU:HD11	1:77:A:PHE:HD2	3	0.23	0.07	0.22
(1,190)	1:49:A:LEU:HD12	1:77:A:PHE:HD1	3	0.23	0.07	0.22
(1,190)	1:49:A:LEU:HD12	1:77:A:PHE:HD2	3	0.23	0.07	0.22
(1,190)	1:49:A:LEU:HD13	1:77:A:PHE:HD1	3	0.23	0.07	0.22
(1,190)	1:49:A:LEU:HD13	1:77:A:PHE:HD2	3	0.23	0.07	0.22
(1,405)	1:108:A:VAL:H	1:110:A:MET:H	3	0.22	0.06	0.25
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD11	3	0.22	0.03	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD12	3	0.22	0.03	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD13	3	0.22	0.03	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD21	3	0.22	0.03	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD22	3	0.22	0.03	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD23	3	0.22	0.03	0.24
(1,632)	1:156:A:ILE:HD11	1:196:A:ARG:H	3	0.22	0.04	0.21
(1,632)	1:156:A:ILE:HD12	1:196:A:ARG:H	3	0.22	0.04	0.21
(1,632)	1:156:A:ILE:HD13	1:196:A:ARG:H	3	0.22	0.04	0.21
(1,325)	1:81:A:VAL:HG11	1:117:A:ILE:H	3	0.21	0.09	0.15
(1,325)	1:81:A:VAL:HG12	1:117:A:ILE:H	3	0.21	0.09	0.15
(1,325)	1:81:A:VAL:HG13	1:117:A:ILE:H	3	0.21	0.09	0.15
(1,325)	1:81:A:VAL:HG21	1:117:A:ILE:H	3	0.21	0.09	0.15
(1,325)	1:81:A:VAL:HG22	1:117:A:ILE:H	3	0.21	0.09	0.15
(1,325)	1:81:A:VAL:HG23	1:117:A:ILE:H	3	0.21	0.09	0.15
(1,650)	1:157:A:VAL:H	1:183:A:SER:H	3	0.21	0.05	0.21
(1,668)	1:159:A:VAL:HG11	1:175:A:PHE:H	3	0.21	0.04	0.19
(1,668)	1:159:A:VAL:HG12	1:175:A:PHE:H	3	0.21	0.04	0.19
(1,668)	1:159:A:VAL:HG13	1:175:A:PHE:H	3	0.21	0.04	0.19
(1,668)	1:159:A:VAL:HG21	1:175:A:PHE:H	3	0.21	0.04	0.19
(1,668)	1:159:A:VAL:HG22	1:175:A:PHE:H	3	0.21	0.04	0.19
(1,668)	1:159:A:VAL:HG23	1:175:A:PHE:H	3	0.21	0.04	0.19
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG11	3	0.2	0.05	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG12	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG13	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG21	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG22	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG23	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG11	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG12	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG13	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG21	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG22	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG23	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG11	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG12	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG13	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG21	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG22	3	0.2	0.05	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG23	3	0.2	0.05	0.23
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD11	3	0.19	0.05	0.16
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD12	3	0.19	0.05	0.16
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD13	3	0.19	0.05	0.16
(1,447)	1:117:A:ILE:HD11	1:118:A:GLY:H	3	0.19	0.04	0.21
(1,447)	1:117:A:ILE:HD12	1:118:A:GLY:H	3	0.19	0.04	0.21
(1,447)	1:117:A:ILE:HD13	1:118:A:GLY:H	3	0.19	0.04	0.21
(1,660)	1:159:A:VAL:HG11	1:169:A:GLN:H	3	0.19	0.06	0.23
(1,660)	1:159:A:VAL:HG12	1:169:A:GLN:H	3	0.19	0.06	0.23
(1,660)	1:159:A:VAL:HG13	1:169:A:GLN:H	3	0.19	0.06	0.23
(1,660)	1:159:A:VAL:HG21	1:169:A:GLN:H	3	0.19	0.06	0.23
(1,660)	1:159:A:VAL:HG22	1:169:A:GLN:H	3	0.19	0.06	0.23
(1,660)	1:159:A:VAL:HG23	1:169:A:GLN:H	3	0.19	0.06	0.23
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG21	3	0.19	0.08	0.15
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG22	3	0.19	0.08	0.15
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG23	3	0.19	0.08	0.15
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD11	3	0.19	0.05	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD12	3	0.19	0.05	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD13	3	0.19	0.05	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD21	3	0.19	0.05	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD22	3	0.19	0.05	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD23	3	0.19	0.05	0.21
(1,633)	1:156:A:ILE:HD11	1:197:A:ALA:H	3	0.19	0.12	0.11
(1,633)	1:156:A:ILE:HD12	1:197:A:ALA:H	3	0.19	0.12	0.11
(1,633)	1:156:A:ILE:HD13	1:197:A:ALA:H	3	0.19	0.12	0.11
(1,597)	1:149:A:LEU:H	1:153:A:LYS:H	3	0.19	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,19)	1:30:A:ALA:H	1:133:A:SER:H	3	0.18	0.07	0.15
(1,31)	1:31:A:LEU:H	1:135:A:LEU:H	3	0.18	0.05	0.2
(1,526)	1:138:A:SER:H	1:157:A:VAL:H	3	0.17	0.05	0.14
(1,529)	1:139:A:HIS:H	1:140:A:ALA:H	3	0.17	0.04	0.16
(1,203)	1:51:A:ASP:H	1:53:A:PHE:H	3	0.16	0.03	0.15
(1,677)	1:161:A:ASP:H	1:163:A:LEU:H	3	0.15	0.01	0.15
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD11	3	0.15	0.02	0.14
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD12	3	0.15	0.02	0.14
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD13	3	0.15	0.02	0.14
(1,6)	1:25:A:ILE:H	1:27:A:GLU:H	3	0.14	0.03	0.14
(1,294)	1:67:A:ILE:HD11	1:69:A:PHE:HD1	3	0.13	0.02	0.14
(1,294)	1:67:A:ILE:HD11	1:69:A:PHE:HD2	3	0.13	0.02	0.14
(1,294)	1:67:A:ILE:HD12	1:69:A:PHE:HD1	3	0.13	0.02	0.14
(1,294)	1:67:A:ILE:HD12	1:69:A:PHE:HD2	3	0.13	0.02	0.14
(1,294)	1:67:A:ILE:HD13	1:69:A:PHE:HD1	3	0.13	0.02	0.14
(1,294)	1:67:A:ILE:HD13	1:69:A:PHE:HD2	3	0.13	0.02	0.14
(1,473)	1:129:A:ILE:H	1:133:A:SER:H	3	0.13	0.02	0.12
(1,649)	1:157:A:VAL:HG21	1:182:A:TRP:H	2	0.48	0.12	0.48
(1,649)	1:157:A:VAL:HG22	1:182:A:TRP:H	2	0.48	0.12	0.48
(1,649)	1:157:A:VAL:HG23	1:182:A:TRP:H	2	0.48	0.12	0.48
(1,576)	1:146:A:LEU:HD11	1:150:A:ARG:H	2	0.39	0.01	0.39
(1,576)	1:146:A:LEU:HD12	1:150:A:ARG:H	2	0.39	0.01	0.39
(1,576)	1:146:A:LEU:HD13	1:150:A:ARG:H	2	0.39	0.01	0.39
(1,576)	1:146:A:LEU:HD21	1:150:A:ARG:H	2	0.39	0.01	0.39
(1,576)	1:146:A:LEU:HD22	1:150:A:ARG:H	2	0.39	0.01	0.39
(1,576)	1:146:A:LEU:HD23	1:150:A:ARG:H	2	0.39	0.01	0.39
(1,55)	1:32:A:PHE:HD1	1:136:A:VAL:HG21	2	0.36	0.04	0.36
(1,55)	1:32:A:PHE:HD1	1:136:A:VAL:HG22	2	0.36	0.04	0.36
(1,55)	1:32:A:PHE:HD1	1:136:A:VAL:HG23	2	0.36	0.04	0.36
(1,55)	1:32:A:PHE:HD2	1:136:A:VAL:HG21	2	0.36	0.04	0.36
(1,55)	1:32:A:PHE:HD2	1:136:A:VAL:HG22	2	0.36	0.04	0.36
(1,55)	1:32:A:PHE:HD2	1:136:A:VAL:HG23	2	0.36	0.04	0.36
(1,760)	1:181:A:VAL:HG21	1:183:A:SER:H	2	0.35	0.07	0.35
(1,760)	1:181:A:VAL:HG22	1:183:A:SER:H	2	0.35	0.07	0.35
(1,760)	1:181:A:VAL:HG23	1:183:A:SER:H	2	0.35	0.07	0.35
(1,37)	1:31:A:LEU:HD11	1:53:A:PHE:HD1	2	0.34	0.0	0.34
(1,37)	1:31:A:LEU:HD11	1:53:A:PHE:HD2	2	0.34	0.0	0.34
(1,37)	1:31:A:LEU:HD12	1:53:A:PHE:HD1	2	0.34	0.0	0.34
(1,37)	1:31:A:LEU:HD12	1:53:A:PHE:HD2	2	0.34	0.0	0.34
(1,37)	1:31:A:LEU:HD13	1:53:A:PHE:HD1	2	0.34	0.0	0.34
(1,37)	1:31:A:LEU:HD13	1:53:A:PHE:HD2	2	0.34	0.0	0.34
(1,368)	1:95:A:ILE:HD11	1:98:A:PHE:H	2	0.34	0.03	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,368)	1:95:A:ILE:HD12	1:98:A:PHE:H	2	0.34	0.03	0.34
(1,368)	1:95:A:ILE:HD13	1:98:A:PHE:H	2	0.34	0.03	0.34
(1,35)	1:31:A:LEU:HD11	1:32:A:PHE:H	2	0.32	0.08	0.32
(1,35)	1:31:A:LEU:HD12	1:32:A:PHE:H	2	0.32	0.08	0.32
(1,35)	1:31:A:LEU:HD13	1:32:A:PHE:H	2	0.32	0.08	0.32
(1,35)	1:31:A:LEU:HD21	1:32:A:PHE:H	2	0.32	0.08	0.32
(1,35)	1:31:A:LEU:HD22	1:32:A:PHE:H	2	0.32	0.08	0.32
(1,35)	1:31:A:LEU:HD23	1:32:A:PHE:H	2	0.32	0.08	0.32
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG11	2	0.32	0.02	0.32
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG12	2	0.32	0.02	0.32
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG13	2	0.32	0.02	0.32
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG21	2	0.32	0.02	0.32
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG22	2	0.32	0.02	0.32
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG23	2	0.32	0.02	0.32
(1,873)	1:211:A:ASN:H	1:211:A:ASN:HD22	2	0.32	0.02	0.32
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG11	2	0.32	0.12	0.32
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG12	2	0.32	0.12	0.32
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG13	2	0.32	0.12	0.32
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG21	2	0.32	0.12	0.32
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG22	2	0.32	0.12	0.32
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG23	2	0.32	0.12	0.32
(1,358)	1:89:A:GLU:H	1:106:A:GLN:H	2	0.32	0.04	0.32
(1,546)	1:141:A:GLY:H	1:157:A:VAL:HG11	2	0.3	0.02	0.3
(1,546)	1:141:A:GLY:H	1:157:A:VAL:HG12	2	0.3	0.02	0.3
(1,546)	1:141:A:GLY:H	1:157:A:VAL:HG13	2	0.3	0.02	0.3
(1,420)	1:109:A:LEU:HD11	1:114:A:LEU:H	2	0.29	0.18	0.29
(1,420)	1:109:A:LEU:HD12	1:114:A:LEU:H	2	0.29	0.18	0.29
(1,420)	1:109:A:LEU:HD13	1:114:A:LEU:H	2	0.29	0.18	0.29
(1,420)	1:109:A:LEU:HD21	1:114:A:LEU:H	2	0.29	0.18	0.29
(1,420)	1:109:A:LEU:HD22	1:114:A:LEU:H	2	0.29	0.18	0.29
(1,420)	1:109:A:LEU:HD23	1:114:A:LEU:H	2	0.29	0.18	0.29
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD11	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD12	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD13	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD21	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD22	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD23	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD11	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD12	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD13	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD21	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD22	2	0.29	0.02	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD23	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD11	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD12	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD13	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD21	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD22	2	0.29	0.02	0.29
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD23	2	0.29	0.02	0.29
(1,772)	1:182:A:TRP:HE1	1:203:A:LEU:H	2	0.28	0.13	0.28
(1,51)	1:32:A:PHE:H	1:134:A:ASP:H	2	0.28	0.1	0.28
(1,62)	1:32:A:PHE:H	1:66:A:ILE:HD11	2	0.28	0.08	0.28
(1,62)	1:32:A:PHE:H	1:66:A:ILE:HD12	2	0.28	0.08	0.28
(1,62)	1:32:A:PHE:H	1:66:A:ILE:HD13	2	0.28	0.08	0.28
(1,534)	1:139:A:HIS:H	1:157:A:VAL:HG21	2	0.28	0.12	0.28
(1,534)	1:139:A:HIS:H	1:157:A:VAL:HG22	2	0.28	0.12	0.28
(1,534)	1:139:A:HIS:H	1:157:A:VAL:HG23	2	0.28	0.12	0.28
(1,379)	1:104:A:ALA:HB1	1:118:A:GLY:H	2	0.27	0.15	0.27
(1,379)	1:104:A:ALA:HB2	1:118:A:GLY:H	2	0.27	0.15	0.27
(1,379)	1:104:A:ALA:HB3	1:118:A:GLY:H	2	0.27	0.15	0.27
(1,400)	1:108:A:VAL:H	1:108:A:VAL:HG21	2	0.26	0.03	0.26
(1,400)	1:108:A:VAL:H	1:108:A:VAL:HG22	2	0.26	0.03	0.26
(1,400)	1:108:A:VAL:H	1:108:A:VAL:HG23	2	0.26	0.03	0.26
(1,191)	1:49:A:LEU:HD21	1:77:A:PHE:HD1	2	0.26	0.14	0.26
(1,191)	1:49:A:LEU:HD21	1:77:A:PHE:HD2	2	0.26	0.14	0.26
(1,191)	1:49:A:LEU:HD22	1:77:A:PHE:HD1	2	0.26	0.14	0.26
(1,191)	1:49:A:LEU:HD22	1:77:A:PHE:HD2	2	0.26	0.14	0.26
(1,191)	1:49:A:LEU:HD23	1:77:A:PHE:HD1	2	0.26	0.14	0.26
(1,191)	1:49:A:LEU:HD23	1:77:A:PHE:HD2	2	0.26	0.14	0.26
(1,288)	1:66:A:ILE:H	1:68:A:GLN:H	2	0.26	0.08	0.26
(1,17)	1:29:A:LYS:H	1:63:A:VAL:HG11	2	0.25	0.02	0.25
(1,17)	1:29:A:LYS:H	1:63:A:VAL:HG12	2	0.25	0.02	0.25
(1,17)	1:29:A:LYS:H	1:63:A:VAL:HG13	2	0.25	0.02	0.25
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG11	2	0.25	0.04	0.25
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG12	2	0.25	0.04	0.25
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG13	2	0.25	0.04	0.25
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG21	2	0.25	0.04	0.25
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG22	2	0.25	0.04	0.25
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG23	2	0.25	0.04	0.25
(1,53)	1:32:A:PHE:HD1	1:136:A:VAL:H	2	0.24	0.02	0.24
(1,53)	1:32:A:PHE:HD2	1:136:A:VAL:H	2	0.24	0.02	0.24
(1,353)	1:87:A:GLN:H	1:109:A:LEU:H	2	0.24	0.07	0.24
(1,247)	1:57:A:LEU:HD11	1:62:A:PHE:HE1	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD11	1:62:A:PHE:HE2	2	0.22	0.08	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,247)	1:57:A:LEU:HD12	1:62:A:PHE:HE1	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD12	1:62:A:PHE:HE2	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD13	1:62:A:PHE:HE1	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD13	1:62:A:PHE:HE2	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD21	1:62:A:PHE:HE1	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD21	1:62:A:PHE:HE2	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD22	1:62:A:PHE:HE1	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD22	1:62:A:PHE:HE2	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD23	1:62:A:PHE:HE1	2	0.22	0.08	0.22
(1,247)	1:57:A:LEU:HD23	1:62:A:PHE:HE2	2	0.22	0.08	0.22
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD11	2	0.22	0.04	0.22
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD12	2	0.22	0.04	0.22
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD13	2	0.22	0.04	0.22
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD21	2	0.22	0.04	0.22
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD22	2	0.22	0.04	0.22
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD23	2	0.22	0.04	0.22
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG11	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG12	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG13	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG21	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG22	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG23	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG11	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG12	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG13	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG21	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG22	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG23	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG11	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG12	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG13	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG21	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG22	2	0.22	0.12	0.22
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG23	2	0.22	0.12	0.22
(1,782)	1:184:A:CYS:HG	1:187:A:THR:H	2	0.22	0.06	0.22
(1,95)	1:35:A:CYS:H	1:67:A:ILE:HG21	2	0.22	0.07	0.22
(1,95)	1:35:A:CYS:H	1:67:A:ILE:HG22	2	0.22	0.07	0.22
(1,95)	1:35:A:CYS:H	1:67:A:ILE:HG23	2	0.22	0.07	0.22
(1,291)	1:67:A:ILE:H	1:118:A:GLY:H	2	0.21	0.07	0.21
(1,463)	1:127:A:SER:H	1:130:A:ARG:H	2	0.21	0.07	0.21
(1,577)	1:146:A:LEU:HD11	1:175:A:PHE:HE1	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD11	1:175:A:PHE:HE2	2	0.21	0.1	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,577)	1:146:A:LEU:HD12	1:175:A:PHE:HE1	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD12	1:175:A:PHE:HE2	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD13	1:175:A:PHE:HE1	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD13	1:175:A:PHE:HE2	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD21	1:175:A:PHE:HE1	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD21	1:175:A:PHE:HE2	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD22	1:175:A:PHE:HE1	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD22	1:175:A:PHE:HE2	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD23	1:175:A:PHE:HE1	2	0.21	0.1	0.21
(1,577)	1:146:A:LEU:HD23	1:175:A:PHE:HE2	2	0.21	0.1	0.21
(1,841)	1:195:A:LEU:HD11	1:199:A:GLN:H	2	0.21	0.0	0.21
(1,841)	1:195:A:LEU:HD12	1:199:A:GLN:H	2	0.21	0.0	0.21
(1,841)	1:195:A:LEU:HD13	1:199:A:GLN:H	2	0.21	0.0	0.21
(1,841)	1:195:A:LEU:HD21	1:199:A:GLN:H	2	0.21	0.0	0.21
(1,841)	1:195:A:LEU:HD22	1:199:A:GLN:H	2	0.21	0.0	0.21
(1,841)	1:195:A:LEU:HD23	1:199:A:GLN:H	2	0.21	0.0	0.21
(1,295)	1:67:A:ILE:HD11	1:69:A:PHE:HE1	2	0.2	0.08	0.2
(1,295)	1:67:A:ILE:HD11	1:69:A:PHE:HE2	2	0.2	0.08	0.2
(1,295)	1:67:A:ILE:HD12	1:69:A:PHE:HE1	2	0.2	0.08	0.2
(1,295)	1:67:A:ILE:HD12	1:69:A:PHE:HE2	2	0.2	0.08	0.2
(1,295)	1:67:A:ILE:HD13	1:69:A:PHE:HE1	2	0.2	0.08	0.2
(1,295)	1:67:A:ILE:HD13	1:69:A:PHE:HE2	2	0.2	0.08	0.2
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD11	2	0.2	0.09	0.2
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD12	2	0.2	0.09	0.2
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD13	2	0.2	0.09	0.2
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD21	2	0.2	0.09	0.2
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD22	2	0.2	0.09	0.2
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD23	2	0.2	0.09	0.2
(1,326)	1:81:A:VAL:HG11	1:118:A:GLY:H	2	0.2	0.02	0.2
(1,326)	1:81:A:VAL:HG12	1:118:A:GLY:H	2	0.2	0.02	0.2
(1,326)	1:81:A:VAL:HG13	1:118:A:GLY:H	2	0.2	0.02	0.2
(1,326)	1:81:A:VAL:HG21	1:118:A:GLY:H	2	0.2	0.02	0.2
(1,326)	1:81:A:VAL:HG22	1:118:A:GLY:H	2	0.2	0.02	0.2
(1,326)	1:81:A:VAL:HG23	1:118:A:GLY:H	2	0.2	0.02	0.2
(1,821)	1:191:A:LEU:HD21	1:194:A:GLY:H	2	0.2	0.04	0.2
(1,821)	1:191:A:LEU:HD22	1:194:A:GLY:H	2	0.2	0.04	0.2
(1,821)	1:191:A:LEU:HD23	1:194:A:GLY:H	2	0.2	0.04	0.2
(1,537)	1:140:A:ALA:H	1:141:A:GLY:H	2	0.18	0.05	0.18
(1,778)	1:184:A:CYS:H	1:184:A:CYS:HG	2	0.18	0.05	0.18
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG11	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG12	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG13	2	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG21	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG22	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG23	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG11	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG12	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG13	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG21	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG22	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG23	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG11	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG12	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG13	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG21	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG22	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG23	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG11	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG12	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG13	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG21	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG22	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG23	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG11	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG12	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG13	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG21	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG22	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG23	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG11	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG12	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG13	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG21	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG22	2	0.18	0.03	0.18
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG23	2	0.18	0.03	0.18
(1,270)	1:63:A:VAL:H	1:65:A:LEU:H	2	0.17	0.04	0.17
(1,389)	1:106:A:GLN:H	1:118:A:GLY:H	2	0.16	0.06	0.16
(1,412)	1:108:A:VAL:HG21	1:115:A:LYS:H	2	0.16	0.01	0.16
(1,412)	1:108:A:VAL:HG22	1:115:A:LYS:H	2	0.16	0.01	0.16
(1,412)	1:108:A:VAL:HG23	1:115:A:LYS:H	2	0.16	0.01	0.16
(1,494)	1:135:A:LEU:H	1:137:A:ILE:H	2	0.16	0.06	0.16
(1,170)	1:49:A:LEU:HD11	1:109:A:LEU:H	2	0.16	0.03	0.16
(1,170)	1:49:A:LEU:HD12	1:109:A:LEU:H	2	0.16	0.03	0.16
(1,170)	1:49:A:LEU:HD13	1:109:A:LEU:H	2	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,170)	1:49:A:LEU:HD21	1:109:A:LEU:H	2	0.16	0.03	0.16
(1,170)	1:49:A:LEU:HD22	1:109:A:LEU:H	2	0.16	0.03	0.16
(1,170)	1:49:A:LEU:HD23	1:109:A:LEU:H	2	0.16	0.03	0.16
(1,690)	1:170:A:GLN:H	1:173:A:ASP:H	2	0.16	0.05	0.16
(1,802)	1:188:A:GLU:H	1:192:A:ILE:HD11	2	0.16	0.03	0.16
(1,802)	1:188:A:GLU:H	1:192:A:ILE:HD12	2	0.16	0.03	0.16
(1,802)	1:188:A:GLU:H	1:192:A:ILE:HD13	2	0.16	0.03	0.16
(1,427)	1:110:A:MET:H	1:114:A:LEU:H	2	0.15	0.02	0.15
(1,63)	1:33:A:VAL:HG11	1:137:A:ILE:H	2	0.15	0.0	0.15
(1,63)	1:33:A:VAL:HG12	1:137:A:ILE:H	2	0.15	0.0	0.15
(1,63)	1:33:A:VAL:HG13	1:137:A:ILE:H	2	0.15	0.0	0.15
(1,63)	1:33:A:VAL:HG21	1:137:A:ILE:H	2	0.15	0.0	0.15
(1,63)	1:33:A:VAL:HG22	1:137:A:ILE:H	2	0.15	0.0	0.15
(1,63)	1:33:A:VAL:HG23	1:137:A:ILE:H	2	0.15	0.0	0.15
(1,774)	1:182:A:TRP:H	1:203:A:LEU:HD11	2	0.15	0.02	0.15
(1,774)	1:182:A:TRP:H	1:203:A:LEU:HD12	2	0.15	0.02	0.15
(1,774)	1:182:A:TRP:H	1:203:A:LEU:HD13	2	0.15	0.02	0.15
(1,208)	1:52:A:GLU:H	1:55:A:GLN:H	2	0.14	0.04	0.14
(1,338)	1:81:A:VAL:HG11	1:98:A:PHE:HD1	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG11	1:98:A:PHE:HD2	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG12	1:98:A:PHE:HD1	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG12	1:98:A:PHE:HD2	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG13	1:98:A:PHE:HD1	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG13	1:98:A:PHE:HD2	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG21	1:98:A:PHE:HD1	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG21	1:98:A:PHE:HD2	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG22	1:98:A:PHE:HD1	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG22	1:98:A:PHE:HD2	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG23	1:98:A:PHE:HD1	2	0.14	0.01	0.14
(1,338)	1:81:A:VAL:HG23	1:98:A:PHE:HD2	2	0.14	0.01	0.14
(1,511)	1:136:A:VAL:H	1:156:A:ILE:HD11	2	0.14	0.02	0.14
(1,511)	1:136:A:VAL:H	1:156:A:ILE:HD12	2	0.14	0.02	0.14
(1,511)	1:136:A:VAL:H	1:156:A:ILE:HD13	2	0.14	0.02	0.14
(1,652)	1:157:A:VAL:H	1:184:A:CYS:HG	2	0.13	0.03	0.13
(1,731)	1:176:A:VAL:HG11	1:183:A:SER:H	2	0.13	0.01	0.13
(1,731)	1:176:A:VAL:HG12	1:183:A:SER:H	2	0.13	0.01	0.13
(1,731)	1:176:A:VAL:HG13	1:183:A:SER:H	2	0.13	0.01	0.13
(1,731)	1:176:A:VAL:HG21	1:183:A:SER:H	2	0.13	0.01	0.13
(1,731)	1:176:A:VAL:HG22	1:183:A:SER:H	2	0.13	0.01	0.13
(1,731)	1:176:A:VAL:HG23	1:183:A:SER:H	2	0.13	0.01	0.13
(1,859)	1:200:A:THR:H	1:201:A:GLU:H	2	0.13	0.02	0.13
(1,586)	1:148:A:SER:H	1:152:A:ASN:H	2	0.12	0.02	0.12

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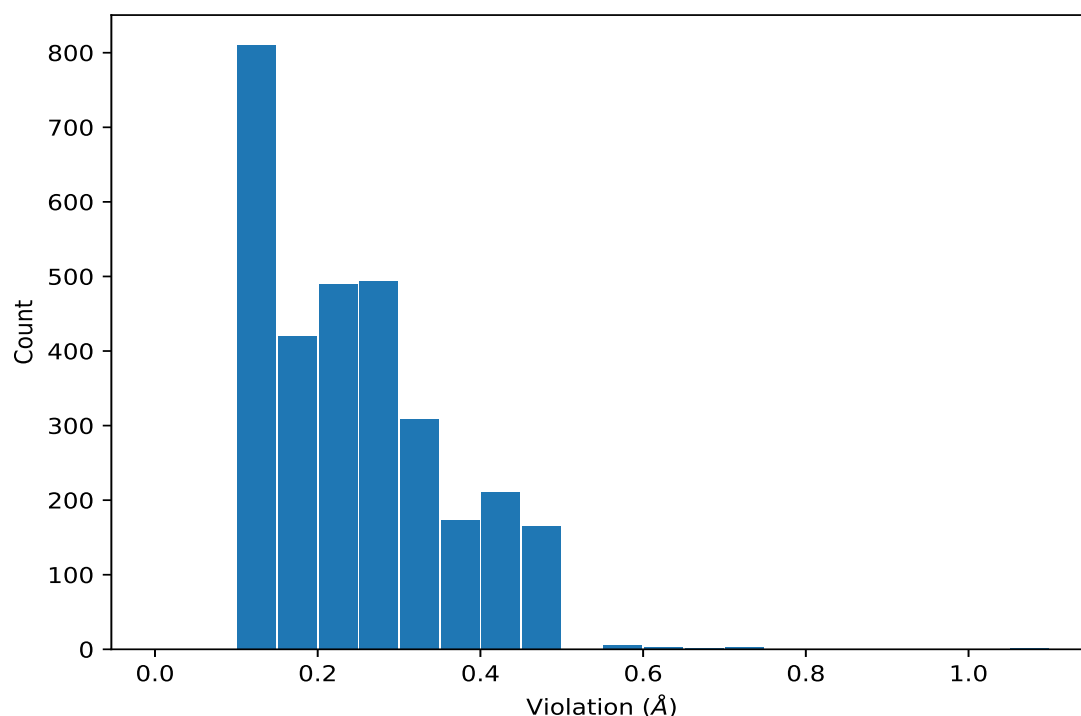
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,863)	1:203:A:LEU:H	1:203:A:LEU:HD21	2	0.12	0.01	0.12
(1,863)	1:203:A:LEU:H	1:203:A:LEU:HD22	2	0.12	0.01	0.12
(1,863)	1:203:A:LEU:H	1:203:A:LEU:HD23	2	0.12	0.01	0.12
(1,205)	1:51:A:ASP:H	1:55:A:GLN:H	2	0.12	0.01	0.12
(1,482)	1:131:A:ASP:H	1:133:A:SER:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:30:A:ALA:H	1:63:A:VAL:H	9	1.09
(1,748)	1:179:A:GLY:H	1:203:A:LEU:HD21	2	0.72
(1,748)	1:179:A:GLY:H	1:203:A:LEU:HD22	2	0.72
(1,748)	1:179:A:GLY:H	1:203:A:LEU:HD23	2	0.72
(1,226)	1:55:A:GLN:H	1:58:A:ILE:HB	7	0.66
(1,649)	1:157:A:VAL:HG21	1:182:A:TRP:H	3	0.61
(1,649)	1:157:A:VAL:HG22	1:182:A:TRP:H	3	0.61
(1,649)	1:157:A:VAL:HG23	1:182:A:TRP:H	3	0.61
(1,110)	1:39:A:VAL:HG21	1:98:A:PHE:HE1	5	0.57
(1,110)	1:39:A:VAL:HG21	1:98:A:PHE:HE2	5	0.57
(1,110)	1:39:A:VAL:HG22	1:98:A:PHE:HE1	5	0.57
(1,110)	1:39:A:VAL:HG22	1:98:A:PHE:HE2	5	0.57
(1,110)	1:39:A:VAL:HG23	1:98:A:PHE:HE1	5	0.57
(1,110)	1:39:A:VAL:HG23	1:98:A:PHE:HE2	5	0.57
(1,410)	1:108:A:VAL:HG11	1:114:A:LEU:H	7	0.48
(1,410)	1:108:A:VAL:HG12	1:114:A:LEU:H	7	0.48
(1,410)	1:108:A:VAL:HG13	1:114:A:LEU:H	7	0.48
(1,410)	1:108:A:VAL:HG21	1:114:A:LEU:H	7	0.48
(1,410)	1:108:A:VAL:HG22	1:114:A:LEU:H	7	0.48
(1,410)	1:108:A:VAL:HG23	1:114:A:LEU:H	7	0.48
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG11	6	0.48
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG12	6	0.48
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG13	6	0.48
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG21	6	0.48
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG22	6	0.48
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG23	6	0.48
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG11	6	0.48
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG12	6	0.48
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG13	6	0.48
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG21	6	0.48
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG22	6	0.48
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG23	6	0.48
(1,761)	1:181:A:VAL:H	1:183:A:SER:H	4	0.47
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG21	7	0.47
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG22	7	0.47
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG23	7	0.47
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG11	2	0.47
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG12	2	0.47
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG13	2	0.47
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG21	2	0.47
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG22	2	0.47
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG23	2	0.47
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG11	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG12	2	0.47
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG13	2	0.47
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG21	2	0.47
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG22	2	0.47
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG23	2	0.47
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG11	2	0.47
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG12	2	0.47
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG13	2	0.47
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG21	2	0.47
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG22	2	0.47
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG23	2	0.47
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG11	2	0.47
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG12	2	0.47
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG13	2	0.47
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG21	2	0.47
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG22	2	0.47
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG23	2	0.47
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG11	2	0.47
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG12	2	0.47
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG13	2	0.47
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG21	2	0.47
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG22	2	0.47
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG23	2	0.47
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG11	2	0.47
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG12	2	0.47
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG13	2	0.47
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG21	2	0.47
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG22	2	0.47
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG23	2	0.47
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG11	3	0.47
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG12	3	0.47
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG13	3	0.47
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG21	3	0.47
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG22	3	0.47
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG23	3	0.47
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG11	3	0.47
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG12	3	0.47
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG13	3	0.47
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG21	3	0.47
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG22	3	0.47
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG23	3	0.47
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG11	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG12	3	0.47
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG13	3	0.47
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG21	3	0.47
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG22	3	0.47
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG23	3	0.47
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG11	3	0.47
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG12	3	0.47
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG13	3	0.47
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG21	3	0.47
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG22	3	0.47
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG23	3	0.47
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG11	3	0.47
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG12	3	0.47
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG13	3	0.47
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG21	3	0.47
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG22	3	0.47
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG23	3	0.47
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG11	3	0.47
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG12	3	0.47
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG13	3	0.47
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG21	3	0.47
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG22	3	0.47
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG23	3	0.47
(1,101)	1:39:A:VAL:HG11	1:44:A:LEU:H	2	0.47
(1,101)	1:39:A:VAL:HG12	1:44:A:LEU:H	2	0.47
(1,101)	1:39:A:VAL:HG13	1:44:A:LEU:H	2	0.47
(1,101)	1:39:A:VAL:HG21	1:44:A:LEU:H	2	0.47
(1,101)	1:39:A:VAL:HG22	1:44:A:LEU:H	2	0.47
(1,101)	1:39:A:VAL:HG23	1:44:A:LEU:H	2	0.47
(1,420)	1:109:A:LEU:HD11	1:114:A:LEU:H	2	0.46
(1,420)	1:109:A:LEU:HD12	1:114:A:LEU:H	2	0.46
(1,420)	1:109:A:LEU:HD13	1:114:A:LEU:H	2	0.46
(1,420)	1:109:A:LEU:HD21	1:114:A:LEU:H	2	0.46
(1,420)	1:109:A:LEU:HD22	1:114:A:LEU:H	2	0.46
(1,420)	1:109:A:LEU:HD23	1:114:A:LEU:H	2	0.46
(1,359)	1:89:A:GLU:H	1:107:A:TYR:H	3	0.46
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG11	9	0.46
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG12	9	0.46
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG13	9	0.46
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG21	9	0.46
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG22	9	0.46
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG23	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG11	9	0.46
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG12	9	0.46
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG13	9	0.46
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG21	9	0.46
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG22	9	0.46
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG23	9	0.46
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG11	9	0.46
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG12	9	0.46
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG13	9	0.46
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG21	9	0.46
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG22	9	0.46
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG23	9	0.46
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG11	9	0.46
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG12	9	0.46
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG13	9	0.46
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG21	9	0.46
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG22	9	0.46
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG23	9	0.46
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG11	9	0.46
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG12	9	0.46
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG13	9	0.46
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG21	9	0.46
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG22	9	0.46
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG23	9	0.46
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG11	9	0.46
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG12	9	0.46
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG13	9	0.46
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG21	9	0.46
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG22	9	0.46
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG23	9	0.46
(1,193)	1:49:A:LEU:HD11	1:80:A:LEU:H	7	0.46
(1,193)	1:49:A:LEU:HD12	1:80:A:LEU:H	7	0.46
(1,193)	1:49:A:LEU:HD13	1:80:A:LEU:H	7	0.46
(1,193)	1:49:A:LEU:HD21	1:80:A:LEU:H	7	0.46
(1,193)	1:49:A:LEU:HD22	1:80:A:LEU:H	7	0.46
(1,193)	1:49:A:LEU:HD23	1:80:A:LEU:H	7	0.46
(1,168)	1:49:A:LEU:HD11	1:107:A:TYR:H	7	0.46
(1,168)	1:49:A:LEU:HD12	1:107:A:TYR:H	7	0.46
(1,168)	1:49:A:LEU:HD13	1:107:A:TYR:H	7	0.46
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD11	5	0.46
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD12	5	0.46
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD13	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:30:A:ALA:H	1:63:A:VAL:H	3	0.46
(1,337)	1:81:A:VAL:HG11	1:89:A:GLU:H	5	0.45
(1,337)	1:81:A:VAL:HG12	1:89:A:GLU:H	5	0.45
(1,337)	1:81:A:VAL:HG13	1:89:A:GLU:H	5	0.45
(1,337)	1:81:A:VAL:HG21	1:89:A:GLU:H	5	0.45
(1,337)	1:81:A:VAL:HG22	1:89:A:GLU:H	5	0.45
(1,337)	1:81:A:VAL:HG23	1:89:A:GLU:H	5	0.45
(1,1)	1:25:A:ILE:HD11	1:26:A:ILE:H	6	0.45
(1,1)	1:25:A:ILE:HD12	1:26:A:ILE:H	6	0.45
(1,1)	1:25:A:ILE:HD13	1:26:A:ILE:H	6	0.45
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD11	9	0.44
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD12	9	0.44
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD13	9	0.44
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD21	9	0.44
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD22	9	0.44
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD23	9	0.44
(1,506)	1:136:A:VAL:H	1:148:A:SER:H	1	0.44
(1,487)	1:134:A:ASP:H	1:136:A:VAL:H	9	0.44
(1,410)	1:108:A:VAL:HG11	1:114:A:LEU:H	1	0.44
(1,410)	1:108:A:VAL:HG12	1:114:A:LEU:H	1	0.44
(1,410)	1:108:A:VAL:HG13	1:114:A:LEU:H	1	0.44
(1,410)	1:108:A:VAL:HG21	1:114:A:LEU:H	1	0.44
(1,410)	1:108:A:VAL:HG22	1:114:A:LEU:H	1	0.44
(1,410)	1:108:A:VAL:HG23	1:114:A:LEU:H	1	0.44
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG11	6	0.44
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG12	6	0.44
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG13	6	0.44
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG21	6	0.44
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG22	6	0.44
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG23	6	0.44
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG11	6	0.44
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG12	6	0.44
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG13	6	0.44
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG21	6	0.44
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG22	6	0.44
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG23	6	0.44
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG11	6	0.44
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG12	6	0.44
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG13	6	0.44
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG21	6	0.44
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG22	6	0.44
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG23	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG11	6	0.44
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG12	6	0.44
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG13	6	0.44
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG21	6	0.44
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG22	6	0.44
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG23	6	0.44
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG11	6	0.44
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG12	6	0.44
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG13	6	0.44
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG21	6	0.44
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG22	6	0.44
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG23	6	0.44
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG11	6	0.44
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG12	6	0.44
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG13	6	0.44
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG21	6	0.44
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG22	6	0.44
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG23	6	0.44
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG11	1	0.44
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG12	1	0.44
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG13	1	0.44
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG21	1	0.44
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG22	1	0.44
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG23	1	0.44
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG11	1	0.44
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG12	1	0.44
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG13	1	0.44
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG21	1	0.44
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG22	1	0.44
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG23	1	0.44
(1,227)	1:55:A:GLN:H	1:58:A:ILE:HD11	1	0.44
(1,227)	1:55:A:GLN:H	1:58:A:ILE:HD12	1	0.44
(1,227)	1:55:A:GLN:H	1:58:A:ILE:HD13	1	0.44
(1,724)	1:176:A:VAL:H	1:180:A:TYR:H	8	0.43
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG21	10	0.43
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG22	10	0.43
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG23	10	0.43
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD11	10	0.43
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD12	10	0.43
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD13	10	0.43
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	3	0.43
(1,220)	1:54:A:CYS:H	1:58:A:ILE:H	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:54:A:CYS:H	1:58:A:ILE:H	8	0.43
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG11	7	0.43
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG12	7	0.43
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG13	7	0.43
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG21	7	0.43
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG22	7	0.43
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG23	7	0.43
(1,760)	1:181:A:VAL:HG21	1:183:A:SER:H	7	0.42
(1,760)	1:181:A:VAL:HG22	1:183:A:SER:H	7	0.42
(1,760)	1:181:A:VAL:HG23	1:183:A:SER:H	7	0.42
(1,610)	1:150:A:ARG:H	1:153:A:LYS:H	2	0.42
(1,567)	1:145:A:ILE:HD11	1:171:A:ILE:H	6	0.42
(1,567)	1:145:A:ILE:HD12	1:171:A:ILE:H	6	0.42
(1,567)	1:145:A:ILE:HD13	1:171:A:ILE:H	6	0.42
(1,495)	1:135:A:LEU:HD11	1:153:A:LYS:H	6	0.42
(1,495)	1:135:A:LEU:HD12	1:153:A:LYS:H	6	0.42
(1,495)	1:135:A:LEU:HD13	1:153:A:LYS:H	6	0.42
(1,495)	1:135:A:LEU:HD21	1:153:A:LYS:H	6	0.42
(1,495)	1:135:A:LEU:HD22	1:153:A:LYS:H	6	0.42
(1,495)	1:135:A:LEU:HD23	1:153:A:LYS:H	6	0.42
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	8	0.42
(1,379)	1:104:A:ALA:HB1	1:118:A:GLY:H	1	0.42
(1,379)	1:104:A:ALA:HB2	1:118:A:GLY:H	1	0.42
(1,379)	1:104:A:ALA:HB3	1:118:A:GLY:H	1	0.42
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD11	3	0.42
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD12	3	0.42
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD13	3	0.42
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD21	3	0.42
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD22	3	0.42
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD23	3	0.42
(1,220)	1:54:A:CYS:H	1:58:A:ILE:H	9	0.42
(1,169)	1:49:A:LEU:HD21	1:107:A:TYR:H	10	0.42
(1,169)	1:49:A:LEU:HD22	1:107:A:TYR:H	10	0.42
(1,169)	1:49:A:LEU:HD23	1:107:A:TYR:H	10	0.42
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD11	4	0.42
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD12	4	0.42
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD13	4	0.42
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD11	4	0.42
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD12	4	0.42
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD13	4	0.42
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	7	0.41
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:182:A:TRP:HE1	1:203:A:LEU:H	8	0.41
(1,743)	1:178:A:LEU:H	1:181:A:VAL:H	4	0.41
(1,645)	1:157:A:VAL:H	1:159:A:VAL:HB	1	0.41
(1,635)	1:156:A:ILE:HG21	1:198:A:SER:H	6	0.41
(1,635)	1:156:A:ILE:HG22	1:198:A:SER:H	6	0.41
(1,635)	1:156:A:ILE:HG23	1:198:A:SER:H	6	0.41
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD11	4	0.41
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD12	4	0.41
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD13	4	0.41
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD21	4	0.41
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD22	4	0.41
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD23	4	0.41
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD11	5	0.41
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD12	5	0.41
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD13	5	0.41
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD11	5	0.41
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD12	5	0.41
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD13	5	0.41
(1,55)	1:32:A:PHE:HD1	1:136:A:VAL:HG21	10	0.41
(1,55)	1:32:A:PHE:HD1	1:136:A:VAL:HG22	10	0.41
(1,55)	1:32:A:PHE:HD1	1:136:A:VAL:HG23	10	0.41
(1,55)	1:32:A:PHE:HD2	1:136:A:VAL:HG21	10	0.41
(1,55)	1:32:A:PHE:HD2	1:136:A:VAL:HG22	10	0.41
(1,55)	1:32:A:PHE:HD2	1:136:A:VAL:HG23	10	0.41
(1,21)	1:30:A:ALA:H	1:134:A:ASP:H	4	0.41
(1,867)	1:203:A:LEU:HD11	1:208:A:VAL:H	7	0.4
(1,867)	1:203:A:LEU:HD12	1:208:A:VAL:H	7	0.4
(1,867)	1:203:A:LEU:HD13	1:208:A:VAL:H	7	0.4
(1,867)	1:203:A:LEU:HD21	1:208:A:VAL:H	7	0.4
(1,867)	1:203:A:LEU:HD22	1:208:A:VAL:H	7	0.4
(1,867)	1:203:A:LEU:HD23	1:208:A:VAL:H	7	0.4
(1,742)	1:178:A:LEU:H	1:180:A:TYR:H	1	0.4
(1,741)	1:178:A:LEU:HD11	1:180:A:TYR:H	8	0.4
(1,741)	1:178:A:LEU:HD12	1:180:A:TYR:H	8	0.4
(1,741)	1:178:A:LEU:HD13	1:180:A:TYR:H	8	0.4
(1,741)	1:178:A:LEU:HD21	1:180:A:TYR:H	8	0.4
(1,741)	1:178:A:LEU:HD22	1:180:A:TYR:H	8	0.4
(1,741)	1:178:A:LEU:HD23	1:180:A:TYR:H	8	0.4
(1,576)	1:146:A:LEU:HD11	1:150:A:ARG:H	8	0.4
(1,576)	1:146:A:LEU:HD12	1:150:A:ARG:H	8	0.4
(1,576)	1:146:A:LEU:HD13	1:150:A:ARG:H	8	0.4
(1,576)	1:146:A:LEU:HD21	1:150:A:ARG:H	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:146:A:LEU:HD22	1:150:A:ARG:H	8	0.4
(1,576)	1:146:A:LEU:HD23	1:150:A:ARG:H	8	0.4
(1,310)	1:81:A:VAL:HG11	1:106:A:GLN:H	10	0.4
(1,310)	1:81:A:VAL:HG12	1:106:A:GLN:H	10	0.4
(1,310)	1:81:A:VAL:HG13	1:106:A:GLN:H	10	0.4
(1,310)	1:81:A:VAL:HG21	1:106:A:GLN:H	10	0.4
(1,310)	1:81:A:VAL:HG22	1:106:A:GLN:H	10	0.4
(1,310)	1:81:A:VAL:HG23	1:106:A:GLN:H	10	0.4
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG11	4	0.4
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG12	4	0.4
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG13	4	0.4
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG21	4	0.4
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG22	4	0.4
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG23	4	0.4
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG11	4	0.4
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG12	4	0.4
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG13	4	0.4
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG21	4	0.4
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG22	4	0.4
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG23	4	0.4
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG11	4	0.4
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG12	4	0.4
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG13	4	0.4
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG21	4	0.4
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG22	4	0.4
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG23	4	0.4
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG11	4	0.4
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG12	4	0.4
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG13	4	0.4
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG21	4	0.4
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG22	4	0.4
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG23	4	0.4
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG11	4	0.4
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG12	4	0.4
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG13	4	0.4
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG21	4	0.4
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG22	4	0.4
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG23	4	0.4
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG11	4	0.4
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG12	4	0.4
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG13	4	0.4
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG21	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG22	4	0.4
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG23	4	0.4
(1,240)	1:57:A:LEU:H	1:58:A:ILE:HD11	1	0.4
(1,240)	1:57:A:LEU:H	1:58:A:ILE:HD12	1	0.4
(1,240)	1:57:A:LEU:H	1:58:A:ILE:HD13	1	0.4
(1,35)	1:31:A:LEU:HD11	1:32:A:PHE:H	9	0.4
(1,35)	1:31:A:LEU:HD12	1:32:A:PHE:H	9	0.4
(1,35)	1:31:A:LEU:HD13	1:32:A:PHE:H	9	0.4
(1,35)	1:31:A:LEU:HD21	1:32:A:PHE:H	9	0.4
(1,35)	1:31:A:LEU:HD22	1:32:A:PHE:H	9	0.4
(1,35)	1:31:A:LEU:HD23	1:32:A:PHE:H	9	0.4
(1,775)	1:182:A:TRP:H	1:203:A:LEU:HD21	6	0.39
(1,775)	1:182:A:TRP:H	1:203:A:LEU:HD22	6	0.39
(1,775)	1:182:A:TRP:H	1:203:A:LEU:HD23	6	0.39
(1,724)	1:176:A:VAL:H	1:180:A:TYR:H	5	0.39
(1,610)	1:150:A:ARG:H	1:153:A:LYS:H	9	0.39
(1,534)	1:139:A:HIS:H	1:157:A:VAL:HG21	7	0.39
(1,534)	1:139:A:HIS:H	1:157:A:VAL:HG22	7	0.39
(1,534)	1:139:A:HIS:H	1:157:A:VAL:HG23	7	0.39
(1,411)	1:108:A:VAL:HG11	1:115:A:LYS:H	8	0.39
(1,411)	1:108:A:VAL:HG12	1:115:A:LYS:H	8	0.39
(1,411)	1:108:A:VAL:HG13	1:115:A:LYS:H	8	0.39
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD11	5	0.39
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD12	5	0.39
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD13	5	0.39
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD21	5	0.39
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD22	5	0.39
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD23	5	0.39
(1,191)	1:49:A:LEU:HD21	1:77:A:PHE:HD1	5	0.39
(1,191)	1:49:A:LEU:HD21	1:77:A:PHE:HD2	5	0.39
(1,191)	1:49:A:LEU:HD22	1:77:A:PHE:HD1	5	0.39
(1,191)	1:49:A:LEU:HD22	1:77:A:PHE:HD2	5	0.39
(1,191)	1:49:A:LEU:HD23	1:77:A:PHE:HD1	5	0.39
(1,191)	1:49:A:LEU:HD23	1:77:A:PHE:HD2	5	0.39
(1,180)	1:49:A:LEU:HD11	1:118:A:GLY:H	4	0.39
(1,180)	1:49:A:LEU:HD12	1:118:A:GLY:H	4	0.39
(1,180)	1:49:A:LEU:HD13	1:118:A:GLY:H	4	0.39
(1,180)	1:49:A:LEU:HD21	1:118:A:GLY:H	4	0.39
(1,180)	1:49:A:LEU:HD22	1:118:A:GLY:H	4	0.39
(1,180)	1:49:A:LEU:HD23	1:118:A:GLY:H	4	0.39
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	4	0.39
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:25:A:ILE:HD11	1:27:A:GLU:H	7	0.39
(1,4)	1:25:A:ILE:HD12	1:27:A:GLU:H	7	0.39
(1,4)	1:25:A:ILE:HD13	1:27:A:GLU:H	7	0.39
(1,724)	1:176:A:VAL:H	1:180:A:TYR:H	4	0.38
(1,638)	1:156:A:ILE:HD11	1:201:A:GLU:H	2	0.38
(1,638)	1:156:A:ILE:HD12	1:201:A:GLU:H	2	0.38
(1,638)	1:156:A:ILE:HD13	1:201:A:GLU:H	2	0.38
(1,576)	1:146:A:LEU:HD11	1:150:A:ARG:H	6	0.38
(1,576)	1:146:A:LEU:HD12	1:150:A:ARG:H	6	0.38
(1,576)	1:146:A:LEU:HD13	1:150:A:ARG:H	6	0.38
(1,576)	1:146:A:LEU:HD21	1:150:A:ARG:H	6	0.38
(1,576)	1:146:A:LEU:HD22	1:150:A:ARG:H	6	0.38
(1,576)	1:146:A:LEU:HD23	1:150:A:ARG:H	6	0.38
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD11	7	0.38
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD12	7	0.38
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD13	7	0.38
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	2	0.38
(1,359)	1:89:A:GLU:H	1:107:A:TYR:H	9	0.38
(1,337)	1:81:A:VAL:HG11	1:89:A:GLU:H	6	0.38
(1,337)	1:81:A:VAL:HG12	1:89:A:GLU:H	6	0.38
(1,337)	1:81:A:VAL:HG13	1:89:A:GLU:H	6	0.38
(1,337)	1:81:A:VAL:HG21	1:89:A:GLU:H	6	0.38
(1,337)	1:81:A:VAL:HG22	1:89:A:GLU:H	6	0.38
(1,337)	1:81:A:VAL:HG23	1:89:A:GLU:H	6	0.38
(1,287)	1:66:A:ILE:HG21	1:68:A:GLN:H	8	0.38
(1,287)	1:66:A:ILE:HG22	1:68:A:GLN:H	8	0.38
(1,287)	1:66:A:ILE:HG23	1:68:A:GLN:H	8	0.38
(1,241)	1:57:A:LEU:HD11	1:59:A:GLN:H	2	0.38
(1,241)	1:57:A:LEU:HD12	1:59:A:GLN:H	2	0.38
(1,241)	1:57:A:LEU:HD13	1:59:A:GLN:H	2	0.38
(1,241)	1:57:A:LEU:HD21	1:59:A:GLN:H	2	0.38
(1,241)	1:57:A:LEU:HD22	1:59:A:GLN:H	2	0.38
(1,241)	1:57:A:LEU:HD23	1:59:A:GLN:H	2	0.38
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD11	1	0.38
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD12	1	0.38
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD13	1	0.38
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD21	1	0.38
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD22	1	0.38
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD23	1	0.38
(1,168)	1:49:A:LEU:HD11	1:107:A:TYR:H	4	0.38
(1,168)	1:49:A:LEU:HD12	1:107:A:TYR:H	4	0.38
(1,168)	1:49:A:LEU:HD13	1:107:A:TYR:H	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:44:A:LEU:HD21	1:47:A:CYS:H	7	0.38
(1,132)	1:44:A:LEU:HD22	1:47:A:CYS:H	7	0.38
(1,132)	1:44:A:LEU:HD23	1:47:A:CYS:H	7	0.38
(1,52)	1:32:A:PHE:H	1:135:A:LEU:H	10	0.38
(1,4)	1:25:A:ILE:HD11	1:27:A:GLU:H	6	0.38
(1,4)	1:25:A:ILE:HD12	1:27:A:GLU:H	6	0.38
(1,4)	1:25:A:ILE:HD13	1:27:A:GLU:H	6	0.38
(1,724)	1:176:A:VAL:H	1:180:A:TYR:H	6	0.37
(1,638)	1:156:A:ILE:HD11	1:201:A:GLU:H	1	0.37
(1,638)	1:156:A:ILE:HD12	1:201:A:GLU:H	1	0.37
(1,638)	1:156:A:ILE:HD13	1:201:A:GLU:H	1	0.37
(1,638)	1:156:A:ILE:HD11	1:201:A:GLU:H	5	0.37
(1,638)	1:156:A:ILE:HD12	1:201:A:GLU:H	5	0.37
(1,638)	1:156:A:ILE:HD13	1:201:A:GLU:H	5	0.37
(1,610)	1:150:A:ARG:H	1:153:A:LYS:H	7	0.37
(1,541)	1:140:A:ALA:HB1	1:158:A:CYS:H	9	0.37
(1,541)	1:140:A:ALA:HB2	1:158:A:CYS:H	9	0.37
(1,541)	1:140:A:ALA:HB3	1:158:A:CYS:H	9	0.37
(1,368)	1:95:A:ILE:HD11	1:98:A:PHE:H	8	0.37
(1,368)	1:95:A:ILE:HD12	1:98:A:PHE:H	8	0.37
(1,368)	1:95:A:ILE:HD13	1:98:A:PHE:H	8	0.37
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG11	9	0.37
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG12	9	0.37
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG13	9	0.37
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG21	9	0.37
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG22	9	0.37
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG23	9	0.37
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG11	9	0.37
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG12	9	0.37
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG13	9	0.37
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG21	9	0.37
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG22	9	0.37
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG23	9	0.37
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG11	9	0.37
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG12	9	0.37
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG13	9	0.37
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG21	9	0.37
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG22	9	0.37
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG23	9	0.37
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG11	9	0.37
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG12	9	0.37
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG13	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG21	9	0.37
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG22	9	0.37
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG23	9	0.37
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG11	9	0.37
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG12	9	0.37
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG13	9	0.37
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG21	9	0.37
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG22	9	0.37
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG23	9	0.37
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG11	9	0.37
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG12	9	0.37
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG13	9	0.37
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG21	9	0.37
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG22	9	0.37
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG23	9	0.37
(1,271)	1:64:A:ARG:H	1:115:A:LYS:H	6	0.37
(1,232)	1:56:A:GLU:H	1:58:A:ILE:HB	7	0.37
(1,220)	1:54:A:CYS:H	1:58:A:ILE:H	10	0.37
(1,153)	1:47:A:CYS:H	1:52:A:GLU:H	7	0.37
(1,51)	1:32:A:PHE:H	1:134:A:ASP:H	6	0.37
(1,27)	1:30:A:ALA:H	1:63:A:VAL:H	8	0.37
(1,867)	1:203:A:LEU:HD11	1:208:A:VAL:H	2	0.36
(1,867)	1:203:A:LEU:HD12	1:208:A:VAL:H	2	0.36
(1,867)	1:203:A:LEU:HD13	1:208:A:VAL:H	2	0.36
(1,867)	1:203:A:LEU:HD21	1:208:A:VAL:H	2	0.36
(1,867)	1:203:A:LEU:HD22	1:208:A:VAL:H	2	0.36
(1,867)	1:203:A:LEU:HD23	1:208:A:VAL:H	2	0.36
(1,761)	1:181:A:VAL:H	1:183:A:SER:H	6	0.36
(1,649)	1:157:A:VAL:HG21	1:182:A:TRP:H	10	0.36
(1,649)	1:157:A:VAL:HG22	1:182:A:TRP:H	10	0.36
(1,649)	1:157:A:VAL:HG23	1:182:A:TRP:H	10	0.36
(1,633)	1:156:A:ILE:HD11	1:197:A:ALA:H	1	0.36
(1,633)	1:156:A:ILE:HD12	1:197:A:ALA:H	1	0.36
(1,633)	1:156:A:ILE:HD13	1:197:A:ALA:H	1	0.36
(1,444)	1:116:A:VAL:H	1:118:A:GLY:H	1	0.36
(1,409)	1:108:A:VAL:HG11	1:113:A:LYS:H	1	0.36
(1,409)	1:108:A:VAL:HG12	1:113:A:LYS:H	1	0.36
(1,409)	1:108:A:VAL:HG13	1:113:A:LYS:H	1	0.36
(1,409)	1:108:A:VAL:HG21	1:113:A:LYS:H	1	0.36
(1,409)	1:108:A:VAL:HG22	1:113:A:LYS:H	1	0.36
(1,409)	1:108:A:VAL:HG23	1:113:A:LYS:H	1	0.36
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD11	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD12	3	0.36
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD13	3	0.36
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	6	0.36
(1,380)	1:104:A:ALA:H	1:118:A:GLY:H	4	0.36
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG21	6	0.36
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG22	6	0.36
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG23	6	0.36
(1,358)	1:89:A:GLU:H	1:106:A:GLN:H	5	0.36
(1,184)	1:49:A:LEU:H	1:51:A:ASP:H	2	0.36
(1,83)	1:34:A:THR:H	1:137:A:ILE:H	10	0.36
(1,62)	1:32:A:PHE:H	1:66:A:ILE:HD11	5	0.36
(1,62)	1:32:A:PHE:H	1:66:A:ILE:HD12	5	0.36
(1,62)	1:32:A:PHE:H	1:66:A:ILE:HD13	5	0.36
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD11	1	0.36
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD12	1	0.36
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD13	1	0.36
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG11	7	0.35
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG12	7	0.35
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG13	7	0.35
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG21	7	0.35
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG22	7	0.35
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG23	7	0.35
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG11	7	0.35
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG12	7	0.35
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG13	7	0.35
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG21	7	0.35
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG22	7	0.35
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG23	7	0.35
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG11	7	0.35
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG12	7	0.35
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG13	7	0.35
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG21	7	0.35
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG22	7	0.35
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG23	7	0.35
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	4	0.35
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG21	10	0.35
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG22	10	0.35
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG23	10	0.35
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG11	3	0.35
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG12	3	0.35
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG13	3	0.35
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG21	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG22	3	0.35
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG23	3	0.35
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG11	3	0.35
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG12	3	0.35
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG13	3	0.35
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG21	3	0.35
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG22	3	0.35
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG23	3	0.35
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG11	3	0.35
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG12	3	0.35
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG13	3	0.35
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG21	3	0.35
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG22	3	0.35
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG23	3	0.35
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG11	3	0.35
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG12	3	0.35
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG13	3	0.35
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG21	3	0.35
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG22	3	0.35
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG23	3	0.35
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG11	3	0.35
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG12	3	0.35
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG13	3	0.35
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG21	3	0.35
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG22	3	0.35
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG23	3	0.35
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG11	3	0.35
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG12	3	0.35
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG13	3	0.35
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG21	3	0.35
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG22	3	0.35
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG23	3	0.35
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG11	4	0.35
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG12	4	0.35
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG13	4	0.35
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG21	4	0.35
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG22	4	0.35
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG23	4	0.35
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG11	4	0.35
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG12	4	0.35
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG13	4	0.35
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG21	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG22	4	0.35
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG23	4	0.35
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	3	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD11	9	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD12	9	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD13	9	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD21	9	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD22	9	0.35
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD23	9	0.35
(1,193)	1:49:A:LEU:HD11	1:80:A:LEU:H	6	0.35
(1,193)	1:49:A:LEU:HD12	1:80:A:LEU:H	6	0.35
(1,193)	1:49:A:LEU:HD13	1:80:A:LEU:H	6	0.35
(1,193)	1:49:A:LEU:HD21	1:80:A:LEU:H	6	0.35
(1,193)	1:49:A:LEU:HD22	1:80:A:LEU:H	6	0.35
(1,193)	1:49:A:LEU:HD23	1:80:A:LEU:H	6	0.35
(1,184)	1:49:A:LEU:H	1:51:A:ASP:H	9	0.35
(1,37)	1:31:A:LEU:HD11	1:53:A:PHE:HD1	9	0.35
(1,37)	1:31:A:LEU:HD11	1:53:A:PHE:HD2	9	0.35
(1,37)	1:31:A:LEU:HD12	1:53:A:PHE:HD1	9	0.35
(1,37)	1:31:A:LEU:HD12	1:53:A:PHE:HD2	9	0.35
(1,37)	1:31:A:LEU:HD13	1:53:A:PHE:HD1	9	0.35
(1,37)	1:31:A:LEU:HD13	1:53:A:PHE:HD2	9	0.35
(1,873)	1:211:A:ASN:H	1:211:A:ASN:HD22	8	0.34
(1,867)	1:203:A:LEU:HD11	1:208:A:VAL:H	6	0.34
(1,867)	1:203:A:LEU:HD12	1:208:A:VAL:H	6	0.34
(1,867)	1:203:A:LEU:HD13	1:208:A:VAL:H	6	0.34
(1,867)	1:203:A:LEU:HD21	1:208:A:VAL:H	6	0.34
(1,867)	1:203:A:LEU:HD22	1:208:A:VAL:H	6	0.34
(1,867)	1:203:A:LEU:HD23	1:208:A:VAL:H	6	0.34
(1,771)	1:182:A:TRP:HE1	1:202:A:LYS:H	9	0.34
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG11	7	0.34
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG12	7	0.34
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG13	7	0.34
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG21	7	0.34
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG22	7	0.34
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG23	7	0.34
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG21	5	0.34
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG22	5	0.34
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG23	5	0.34
(1,325)	1:81:A:VAL:HG11	1:117:A:ILE:H	6	0.34
(1,325)	1:81:A:VAL:HG12	1:117:A:ILE:H	6	0.34
(1,325)	1:81:A:VAL:HG13	1:117:A:ILE:H	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:81:A:VAL:HG21	1:117:A:ILE:H	6	0.34
(1,325)	1:81:A:VAL:HG22	1:117:A:ILE:H	6	0.34
(1,325)	1:81:A:VAL:HG23	1:117:A:ILE:H	6	0.34
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	1	0.34
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	2	0.34
(1,180)	1:49:A:LEU:HD11	1:118:A:GLY:H	6	0.34
(1,180)	1:49:A:LEU:HD12	1:118:A:GLY:H	6	0.34
(1,180)	1:49:A:LEU:HD13	1:118:A:GLY:H	6	0.34
(1,180)	1:49:A:LEU:HD21	1:118:A:GLY:H	6	0.34
(1,180)	1:49:A:LEU:HD22	1:118:A:GLY:H	6	0.34
(1,180)	1:49:A:LEU:HD23	1:118:A:GLY:H	6	0.34
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	7	0.34
(1,37)	1:31:A:LEU:HD11	1:53:A:PHE:HD1	7	0.34
(1,37)	1:31:A:LEU:HD11	1:53:A:PHE:HD2	7	0.34
(1,37)	1:31:A:LEU:HD12	1:53:A:PHE:HD1	7	0.34
(1,37)	1:31:A:LEU:HD12	1:53:A:PHE:HD2	7	0.34
(1,37)	1:31:A:LEU:HD13	1:53:A:PHE:HD1	7	0.34
(1,37)	1:31:A:LEU:HD13	1:53:A:PHE:HD2	7	0.34
(1,596)	1:149:A:LEU:HD11	1:153:A:LYS:H	9	0.33
(1,596)	1:149:A:LEU:HD12	1:153:A:LYS:H	9	0.33
(1,596)	1:149:A:LEU:HD13	1:153:A:LYS:H	9	0.33
(1,596)	1:149:A:LEU:HD21	1:153:A:LYS:H	9	0.33
(1,596)	1:149:A:LEU:HD22	1:153:A:LYS:H	9	0.33
(1,596)	1:149:A:LEU:HD23	1:153:A:LYS:H	9	0.33
(1,544)	1:141:A:GLY:H	1:144:A:SER:H	7	0.33
(1,506)	1:136:A:VAL:H	1:148:A:SER:H	8	0.33
(1,359)	1:89:A:GLU:H	1:107:A:TYR:H	8	0.33
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG11	2	0.33
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG12	2	0.33
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG13	2	0.33
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG11	3	0.33
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG12	3	0.33
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG13	3	0.33
(1,288)	1:66:A:ILE:H	1:68:A:GLN:H	7	0.33
(1,263)	1:63:A:VAL:H	1:115:A:LYS:H	7	0.33
(1,184)	1:49:A:LEU:H	1:51:A:ASP:H	10	0.33
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	6	0.33
(1,80)	1:33:A:VAL:H	1:68:A:GLN:H	10	0.33
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD11	8	0.33
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD12	8	0.33
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD13	8	0.33
(1,741)	1:178:A:LEU:HD11	1:180:A:TYR:H	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:178:A:LEU:HD12	1:180:A:TYR:H	4	0.32
(1,741)	1:178:A:LEU:HD13	1:180:A:TYR:H	4	0.32
(1,741)	1:178:A:LEU:HD21	1:180:A:TYR:H	4	0.32
(1,741)	1:178:A:LEU:HD22	1:180:A:TYR:H	4	0.32
(1,741)	1:178:A:LEU:HD23	1:180:A:TYR:H	4	0.32
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG21	8	0.32
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG22	8	0.32
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG23	8	0.32
(1,610)	1:150:A:ARG:H	1:153:A:LYS:H	8	0.32
(1,546)	1:141:A:GLY:H	1:157:A:VAL:HG11	5	0.32
(1,546)	1:141:A:GLY:H	1:157:A:VAL:HG12	5	0.32
(1,546)	1:141:A:GLY:H	1:157:A:VAL:HG13	5	0.32
(1,444)	1:116:A:VAL:H	1:118:A:GLY:H	7	0.32
(1,374)	1:98:A:PHE:HD1	1:116:A:VAL:HG11	10	0.32
(1,374)	1:98:A:PHE:HD1	1:116:A:VAL:HG12	10	0.32
(1,374)	1:98:A:PHE:HD1	1:116:A:VAL:HG13	10	0.32
(1,374)	1:98:A:PHE:HD1	1:116:A:VAL:HG21	10	0.32
(1,374)	1:98:A:PHE:HD1	1:116:A:VAL:HG22	10	0.32
(1,374)	1:98:A:PHE:HD1	1:116:A:VAL:HG23	10	0.32
(1,374)	1:98:A:PHE:HD2	1:116:A:VAL:HG11	10	0.32
(1,374)	1:98:A:PHE:HD2	1:116:A:VAL:HG12	10	0.32
(1,374)	1:98:A:PHE:HD2	1:116:A:VAL:HG13	10	0.32
(1,374)	1:98:A:PHE:HD2	1:116:A:VAL:HG21	10	0.32
(1,374)	1:98:A:PHE:HD2	1:116:A:VAL:HG22	10	0.32
(1,374)	1:98:A:PHE:HD2	1:116:A:VAL:HG23	10	0.32
(1,290)	1:67:A:ILE:H	1:117:A:ILE:HG21	4	0.32
(1,290)	1:67:A:ILE:H	1:117:A:ILE:HG22	4	0.32
(1,290)	1:67:A:ILE:H	1:117:A:ILE:HG23	4	0.32
(1,271)	1:64:A:ARG:H	1:115:A:LYS:H	9	0.32
(1,190)	1:49:A:LEU:HD11	1:77:A:PHE:HD1	4	0.32
(1,190)	1:49:A:LEU:HD11	1:77:A:PHE:HD2	4	0.32
(1,190)	1:49:A:LEU:HD12	1:77:A:PHE:HD1	4	0.32
(1,190)	1:49:A:LEU:HD12	1:77:A:PHE:HD2	4	0.32
(1,190)	1:49:A:LEU:HD13	1:77:A:PHE:HD1	4	0.32
(1,190)	1:49:A:LEU:HD13	1:77:A:PHE:HD2	4	0.32
(1,184)	1:49:A:LEU:H	1:51:A:ASP:H	7	0.32
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	10	0.32
(1,84)	1:34:A:THR:H	1:137:A:ILE:HG21	3	0.32
(1,84)	1:34:A:THR:H	1:137:A:ILE:HG22	3	0.32
(1,84)	1:34:A:THR:H	1:137:A:ILE:HG23	3	0.32
(1,55)	1:32:A:PHE:HD1	1:136:A:VAL:HG21	6	0.32
(1,55)	1:32:A:PHE:HD1	1:136:A:VAL:HG22	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:32:A:PHE:HD1	1:136:A:VAL:HG23	6	0.32
(1,55)	1:32:A:PHE:HD2	1:136:A:VAL:HG21	6	0.32
(1,55)	1:32:A:PHE:HD2	1:136:A:VAL:HG22	6	0.32
(1,55)	1:32:A:PHE:HD2	1:136:A:VAL:HG23	6	0.32
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD11	1	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD12	1	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD13	1	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD21	1	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD22	1	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD23	1	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD11	1	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD12	1	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD13	1	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD21	1	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD22	1	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD23	1	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD11	2	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD12	2	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD13	2	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD21	2	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD22	2	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD23	2	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD11	2	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD12	2	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD13	2	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD21	2	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD22	2	0.31
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD23	2	0.31
(1,874)	1:211:A:ASN:HD21	1:215:A:GLU:H	3	0.31
(1,874)	1:211:A:ASN:HD22	1:215:A:GLU:H	3	0.31
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	3	0.31
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	3	0.31
(1,820)	1:191:A:LEU:HD11	1:194:A:GLY:H	4	0.31
(1,820)	1:191:A:LEU:HD12	1:194:A:GLY:H	4	0.31
(1,820)	1:191:A:LEU:HD13	1:194:A:GLY:H	4	0.31
(1,647)	1:157:A:VAL:H	1:181:A:VAL:HG11	9	0.31
(1,647)	1:157:A:VAL:H	1:181:A:VAL:HG12	9	0.31
(1,647)	1:157:A:VAL:H	1:181:A:VAL:HG13	9	0.31
(1,647)	1:157:A:VAL:H	1:181:A:VAL:HG21	9	0.31
(1,647)	1:157:A:VAL:H	1:181:A:VAL:HG22	9	0.31
(1,647)	1:157:A:VAL:H	1:181:A:VAL:HG23	9	0.31
(1,638)	1:156:A:ILE:HD11	1:201:A:GLU:H	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:156:A:ILE:HD12	1:201:A:GLU:H	8	0.31
(1,638)	1:156:A:ILE:HD13	1:201:A:GLU:H	8	0.31
(1,577)	1:146:A:LEU:HD11	1:175:A:PHE:HE1	7	0.31
(1,577)	1:146:A:LEU:HD11	1:175:A:PHE:HE2	7	0.31
(1,577)	1:146:A:LEU:HD12	1:175:A:PHE:HE1	7	0.31
(1,577)	1:146:A:LEU:HD12	1:175:A:PHE:HE2	7	0.31
(1,577)	1:146:A:LEU:HD13	1:175:A:PHE:HE1	7	0.31
(1,577)	1:146:A:LEU:HD13	1:175:A:PHE:HE2	7	0.31
(1,577)	1:146:A:LEU:HD21	1:175:A:PHE:HE1	7	0.31
(1,577)	1:146:A:LEU:HD21	1:175:A:PHE:HE2	7	0.31
(1,577)	1:146:A:LEU:HD22	1:175:A:PHE:HE1	7	0.31
(1,577)	1:146:A:LEU:HD22	1:175:A:PHE:HE2	7	0.31
(1,577)	1:146:A:LEU:HD23	1:175:A:PHE:HE1	7	0.31
(1,577)	1:146:A:LEU:HD23	1:175:A:PHE:HE2	7	0.31
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD11	3	0.31
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD12	3	0.31
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD13	3	0.31
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD21	3	0.31
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD22	3	0.31
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD23	3	0.31
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD11	3	0.31
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD12	3	0.31
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD13	3	0.31
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD21	3	0.31
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD22	3	0.31
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD23	3	0.31
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD11	3	0.31
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD12	3	0.31
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD13	3	0.31
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD21	3	0.31
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD22	3	0.31
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD23	3	0.31
(1,398)	1:107:A:TYR:H	1:118:A:GLY:H	7	0.31
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	9	0.31
(1,368)	1:95:A:ILE:HD11	1:98:A:PHE:H	5	0.31
(1,368)	1:95:A:ILE:HD12	1:98:A:PHE:H	5	0.31
(1,368)	1:95:A:ILE:HD13	1:98:A:PHE:H	5	0.31
(1,359)	1:89:A:GLU:H	1:107:A:TYR:H	7	0.31
(1,353)	1:87:A:GLN:H	1:109:A:LEU:H	8	0.31
(1,263)	1:63:A:VAL:H	1:115:A:LYS:H	6	0.31
(1,247)	1:57:A:LEU:HD11	1:62:A:PHE:HE1	3	0.31
(1,247)	1:57:A:LEU:HD11	1:62:A:PHE:HE2	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	1:57:A:LEU:HD12	1:62:A:PHE:HE1	3	0.31
(1,247)	1:57:A:LEU:HD12	1:62:A:PHE:HE2	3	0.31
(1,247)	1:57:A:LEU:HD13	1:62:A:PHE:HE1	3	0.31
(1,247)	1:57:A:LEU:HD13	1:62:A:PHE:HE2	3	0.31
(1,247)	1:57:A:LEU:HD21	1:62:A:PHE:HE1	3	0.31
(1,247)	1:57:A:LEU:HD21	1:62:A:PHE:HE2	3	0.31
(1,247)	1:57:A:LEU:HD22	1:62:A:PHE:HE1	3	0.31
(1,247)	1:57:A:LEU:HD22	1:62:A:PHE:HE2	3	0.31
(1,247)	1:57:A:LEU:HD23	1:62:A:PHE:HE1	3	0.31
(1,247)	1:57:A:LEU:HD23	1:62:A:PHE:HE2	3	0.31
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD11	8	0.31
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD12	8	0.31
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD13	8	0.31
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD21	8	0.31
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD22	8	0.31
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD23	8	0.31
(1,164)	1:48:A:VAL:HG11	1:53:A:PHE:H	6	0.31
(1,164)	1:48:A:VAL:HG12	1:53:A:PHE:H	6	0.31
(1,164)	1:48:A:VAL:HG13	1:53:A:PHE:H	6	0.31
(1,164)	1:48:A:VAL:HG21	1:53:A:PHE:H	6	0.31
(1,164)	1:48:A:VAL:HG22	1:53:A:PHE:H	6	0.31
(1,164)	1:48:A:VAL:HG23	1:53:A:PHE:H	6	0.31
(1,164)	1:48:A:VAL:HG11	1:53:A:PHE:H	10	0.31
(1,164)	1:48:A:VAL:HG12	1:53:A:PHE:H	10	0.31
(1,164)	1:48:A:VAL:HG13	1:53:A:PHE:H	10	0.31
(1,164)	1:48:A:VAL:HG21	1:53:A:PHE:H	10	0.31
(1,164)	1:48:A:VAL:HG22	1:53:A:PHE:H	10	0.31
(1,164)	1:48:A:VAL:HG23	1:53:A:PHE:H	10	0.31
(1,132)	1:44:A:LEU:HD21	1:47:A:CYS:H	8	0.31
(1,132)	1:44:A:LEU:HD22	1:47:A:CYS:H	8	0.31
(1,132)	1:44:A:LEU:HD23	1:47:A:CYS:H	8	0.31
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD11	3	0.3
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD12	3	0.3
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD13	3	0.3
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD21	3	0.3
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD22	3	0.3
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD23	3	0.3
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD11	3	0.3
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD12	3	0.3
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD13	3	0.3
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD21	3	0.3
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD22	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD23	3	0.3
(1,873)	1:211:A:ASN:H	1:211:A:ASN:HD22	3	0.3
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG21	3	0.3
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG22	3	0.3
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG23	3	0.3
(1,741)	1:178:A:LEU:HD11	1:180:A:TYR:H	6	0.3
(1,741)	1:178:A:LEU:HD12	1:180:A:TYR:H	6	0.3
(1,741)	1:178:A:LEU:HD13	1:180:A:TYR:H	6	0.3
(1,741)	1:178:A:LEU:HD21	1:180:A:TYR:H	6	0.3
(1,741)	1:178:A:LEU:HD22	1:180:A:TYR:H	6	0.3
(1,741)	1:178:A:LEU:HD23	1:180:A:TYR:H	6	0.3
(1,600)	1:149:A:LEU:H	1:155:A:LEU:HD21	3	0.3
(1,600)	1:149:A:LEU:H	1:155:A:LEU:HD22	3	0.3
(1,600)	1:149:A:LEU:H	1:155:A:LEU:HD23	3	0.3
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD11	7	0.3
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD12	7	0.3
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD13	7	0.3
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD21	7	0.3
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD22	7	0.3
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD23	7	0.3
(1,487)	1:134:A:ASP:H	1:136:A:VAL:H	7	0.3
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG11	10	0.3
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG12	10	0.3
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG13	10	0.3
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG21	10	0.3
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG22	10	0.3
(1,438)	1:115:A:LYS:H	1:116:A:VAL:HG23	10	0.3
(1,400)	1:108:A:VAL:H	1:108:A:VAL:HG21	6	0.3
(1,400)	1:108:A:VAL:H	1:108:A:VAL:HG22	6	0.3
(1,400)	1:108:A:VAL:H	1:108:A:VAL:HG23	6	0.3
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD11	1	0.3
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD12	1	0.3
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD13	1	0.3
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD21	1	0.3
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD22	1	0.3
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD23	1	0.3
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG11	4	0.3
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG12	4	0.3
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG13	4	0.3
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG21	4	0.3
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG22	4	0.3
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG23	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG11	4	0.3
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG12	4	0.3
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG13	4	0.3
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG21	4	0.3
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG22	4	0.3
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG23	4	0.3
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG11	4	0.3
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG12	4	0.3
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG13	4	0.3
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG21	4	0.3
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG22	4	0.3
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG23	4	0.3
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG11	4	0.3
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG12	4	0.3
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG13	4	0.3
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG21	4	0.3
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG22	4	0.3
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG23	4	0.3
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG11	4	0.3
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG12	4	0.3
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG13	4	0.3
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG21	4	0.3
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG22	4	0.3
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG23	4	0.3
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG11	4	0.3
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG12	4	0.3
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG13	4	0.3
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG21	4	0.3
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG22	4	0.3
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG23	4	0.3
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG11	8	0.3
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG12	8	0.3
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG13	8	0.3
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG21	8	0.3
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG22	8	0.3
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG23	8	0.3
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG11	8	0.3
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG12	8	0.3
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG13	8	0.3
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG21	8	0.3
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG22	8	0.3
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG23	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG11	8	0.3
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG12	8	0.3
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG13	8	0.3
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG21	8	0.3
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG22	8	0.3
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG23	8	0.3
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG11	8	0.3
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG12	8	0.3
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG13	8	0.3
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG21	8	0.3
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG22	8	0.3
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG23	8	0.3
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG11	8	0.3
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG12	8	0.3
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG13	8	0.3
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG21	8	0.3
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG22	8	0.3
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG23	8	0.3
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG11	8	0.3
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG12	8	0.3
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG13	8	0.3
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG21	8	0.3
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG22	8	0.3
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG23	8	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG11	5	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG12	5	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG13	5	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG21	5	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG22	5	0.3
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG23	5	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG11	5	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG12	5	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG13	5	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG21	5	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG22	5	0.3
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG23	5	0.3
(1,262)	1:63:A:VAL:HG11	1:115:A:LYS:H	3	0.3
(1,262)	1:63:A:VAL:HG12	1:115:A:LYS:H	3	0.3
(1,262)	1:63:A:VAL:HG13	1:115:A:LYS:H	3	0.3
(1,262)	1:63:A:VAL:HG21	1:115:A:LYS:H	3	0.3
(1,262)	1:63:A:VAL:HG22	1:115:A:LYS:H	3	0.3
(1,262)	1:63:A:VAL:HG23	1:115:A:LYS:H	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:58:A:ILE:HD11	1:61:A:GLY:H	7	0.3
(1,254)	1:58:A:ILE:HD12	1:61:A:GLY:H	7	0.3
(1,254)	1:58:A:ILE:HD13	1:61:A:GLY:H	7	0.3
(1,241)	1:57:A:LEU:HD11	1:59:A:GLN:H	6	0.3
(1,241)	1:57:A:LEU:HD12	1:59:A:GLN:H	6	0.3
(1,241)	1:57:A:LEU:HD13	1:59:A:GLN:H	6	0.3
(1,241)	1:57:A:LEU:HD21	1:59:A:GLN:H	6	0.3
(1,241)	1:57:A:LEU:HD22	1:59:A:GLN:H	6	0.3
(1,241)	1:57:A:LEU:HD23	1:59:A:GLN:H	6	0.3
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	1	0.3
(1,110)	1:39:A:VAL:HG21	1:98:A:PHE:HE1	1	0.3
(1,110)	1:39:A:VAL:HG21	1:98:A:PHE:HE2	1	0.3
(1,110)	1:39:A:VAL:HG22	1:98:A:PHE:HE1	1	0.3
(1,110)	1:39:A:VAL:HG22	1:98:A:PHE:HE2	1	0.3
(1,110)	1:39:A:VAL:HG23	1:98:A:PHE:HE1	1	0.3
(1,110)	1:39:A:VAL:HG23	1:98:A:PHE:HE2	1	0.3
(1,80)	1:33:A:VAL:H	1:68:A:GLN:H	1	0.3
(1,794)	1:187:A:THR:H	1:189:A:THR:H	6	0.29
(1,782)	1:184:A:CYS:HG	1:187:A:THR:H	8	0.29
(1,670)	1:159:A:VAL:HG11	1:181:A:VAL:H	9	0.29
(1,670)	1:159:A:VAL:HG12	1:181:A:VAL:H	9	0.29
(1,670)	1:159:A:VAL:HG13	1:181:A:VAL:H	9	0.29
(1,670)	1:159:A:VAL:HG21	1:181:A:VAL:H	9	0.29
(1,670)	1:159:A:VAL:HG22	1:181:A:VAL:H	9	0.29
(1,670)	1:159:A:VAL:HG23	1:181:A:VAL:H	9	0.29
(1,635)	1:156:A:ILE:HG21	1:198:A:SER:H	1	0.29
(1,635)	1:156:A:ILE:HG22	1:198:A:SER:H	1	0.29
(1,635)	1:156:A:ILE:HG23	1:198:A:SER:H	1	0.29
(1,531)	1:139:A:HIS:H	1:145:A:ILE:HD11	7	0.29
(1,531)	1:139:A:HIS:H	1:145:A:ILE:HD12	7	0.29
(1,531)	1:139:A:HIS:H	1:145:A:ILE:HD13	7	0.29
(1,310)	1:81:A:VAL:HG11	1:106:A:GLN:H	8	0.29
(1,310)	1:81:A:VAL:HG12	1:106:A:GLN:H	8	0.29
(1,310)	1:81:A:VAL:HG13	1:106:A:GLN:H	8	0.29
(1,310)	1:81:A:VAL:HG21	1:106:A:GLN:H	8	0.29
(1,310)	1:81:A:VAL:HG22	1:106:A:GLN:H	8	0.29
(1,310)	1:81:A:VAL:HG23	1:106:A:GLN:H	8	0.29
(1,295)	1:67:A:ILE:HD11	1:69:A:PHE:HE1	6	0.29
(1,295)	1:67:A:ILE:HD11	1:69:A:PHE:HE2	6	0.29
(1,295)	1:67:A:ILE:HD12	1:69:A:PHE:HE1	6	0.29
(1,295)	1:67:A:ILE:HD12	1:69:A:PHE:HE2	6	0.29
(1,295)	1:67:A:ILE:HD13	1:69:A:PHE:HE1	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:67:A:ILE:HD13	1:69:A:PHE:HE2	6	0.29
(1,271)	1:64:A:ARG:H	1:115:A:LYS:H	1	0.29
(1,271)	1:64:A:ARG:H	1:115:A:LYS:H	8	0.29
(1,241)	1:57:A:LEU:HD11	1:59:A:GLN:H	4	0.29
(1,241)	1:57:A:LEU:HD12	1:59:A:GLN:H	4	0.29
(1,241)	1:57:A:LEU:HD13	1:59:A:GLN:H	4	0.29
(1,241)	1:57:A:LEU:HD21	1:59:A:GLN:H	4	0.29
(1,241)	1:57:A:LEU:HD22	1:59:A:GLN:H	4	0.29
(1,241)	1:57:A:LEU:HD23	1:59:A:GLN:H	4	0.29
(1,241)	1:57:A:LEU:HD11	1:59:A:GLN:H	8	0.29
(1,241)	1:57:A:LEU:HD12	1:59:A:GLN:H	8	0.29
(1,241)	1:57:A:LEU:HD13	1:59:A:GLN:H	8	0.29
(1,241)	1:57:A:LEU:HD21	1:59:A:GLN:H	8	0.29
(1,241)	1:57:A:LEU:HD22	1:59:A:GLN:H	8	0.29
(1,241)	1:57:A:LEU:HD23	1:59:A:GLN:H	8	0.29
(1,180)	1:49:A:LEU:HD11	1:118:A:GLY:H	1	0.29
(1,180)	1:49:A:LEU:HD12	1:118:A:GLY:H	1	0.29
(1,180)	1:49:A:LEU:HD13	1:118:A:GLY:H	1	0.29
(1,180)	1:49:A:LEU:HD21	1:118:A:GLY:H	1	0.29
(1,180)	1:49:A:LEU:HD22	1:118:A:GLY:H	1	0.29
(1,180)	1:49:A:LEU:HD23	1:118:A:GLY:H	1	0.29
(1,95)	1:35:A:CYS:H	1:67:A:ILE:HG21	2	0.29
(1,95)	1:35:A:CYS:H	1:67:A:ILE:HG22	2	0.29
(1,95)	1:35:A:CYS:H	1:67:A:ILE:HG23	2	0.29
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG11	1	0.29
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG12	1	0.29
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG13	1	0.29
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG21	1	0.29
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG22	1	0.29
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG23	1	0.29
(1,52)	1:32:A:PHE:H	1:135:A:LEU:H	4	0.29
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD11	7	0.29
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD12	7	0.29
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD13	7	0.29
(1,4)	1:25:A:ILE:HD11	1:27:A:GLU:H	8	0.29
(1,4)	1:25:A:ILE:HD12	1:27:A:GLU:H	8	0.29
(1,4)	1:25:A:ILE:HD13	1:27:A:GLU:H	8	0.29
(1,4)	1:25:A:ILE:HD11	1:27:A:GLU:H	9	0.29
(1,4)	1:25:A:ILE:HD12	1:27:A:GLU:H	9	0.29
(1,4)	1:25:A:ILE:HD13	1:27:A:GLU:H	9	0.29
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD11	5	0.28
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD12	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD13	5	0.28
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD21	5	0.28
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD22	5	0.28
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD23	5	0.28
(1,760)	1:181:A:VAL:HG21	1:183:A:SER:H	3	0.28
(1,760)	1:181:A:VAL:HG22	1:183:A:SER:H	3	0.28
(1,760)	1:181:A:VAL:HG23	1:183:A:SER:H	3	0.28
(1,610)	1:150:A:ARG:H	1:153:A:LYS:H	5	0.28
(1,596)	1:149:A:LEU:HD11	1:153:A:LYS:H	3	0.28
(1,596)	1:149:A:LEU:HD12	1:153:A:LYS:H	3	0.28
(1,596)	1:149:A:LEU:HD13	1:153:A:LYS:H	3	0.28
(1,596)	1:149:A:LEU:HD21	1:153:A:LYS:H	3	0.28
(1,596)	1:149:A:LEU:HD22	1:153:A:LYS:H	3	0.28
(1,596)	1:149:A:LEU:HD23	1:153:A:LYS:H	3	0.28
(1,568)	1:145:A:ILE:HD11	1:172:A:ALA:H	5	0.28
(1,568)	1:145:A:ILE:HD12	1:172:A:ALA:H	5	0.28
(1,568)	1:145:A:ILE:HD13	1:172:A:ALA:H	5	0.28
(1,463)	1:127:A:SER:H	1:130:A:ARG:H	6	0.28
(1,405)	1:108:A:VAL:H	1:110:A:MET:H	6	0.28
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG11	1	0.28
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG12	1	0.28
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG13	1	0.28
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG21	1	0.28
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG22	1	0.28
(1,302)	1:80:A:LEU:HD11	1:116:A:VAL:HG23	1	0.28
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG11	1	0.28
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG12	1	0.28
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG13	1	0.28
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG21	1	0.28
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG22	1	0.28
(1,302)	1:80:A:LEU:HD12	1:116:A:VAL:HG23	1	0.28
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG11	1	0.28
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG12	1	0.28
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG13	1	0.28
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG21	1	0.28
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG22	1	0.28
(1,302)	1:80:A:LEU:HD13	1:116:A:VAL:HG23	1	0.28
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG11	1	0.28
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG12	1	0.28
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG13	1	0.28
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG21	1	0.28
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG22	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:80:A:LEU:HD21	1:116:A:VAL:HG23	1	0.28
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG11	1	0.28
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG12	1	0.28
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG13	1	0.28
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG21	1	0.28
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG22	1	0.28
(1,302)	1:80:A:LEU:HD22	1:116:A:VAL:HG23	1	0.28
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG11	1	0.28
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG12	1	0.28
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG13	1	0.28
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG21	1	0.28
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG22	1	0.28
(1,302)	1:80:A:LEU:HD23	1:116:A:VAL:HG23	1	0.28
(1,291)	1:67:A:ILE:H	1:118:A:GLY:H	2	0.28
(1,220)	1:54:A:CYS:H	1:58:A:ILE:H	2	0.28
(1,169)	1:49:A:LEU:HD21	1:107:A:TYR:H	2	0.28
(1,169)	1:49:A:LEU:HD22	1:107:A:TYR:H	2	0.28
(1,169)	1:49:A:LEU:HD23	1:107:A:TYR:H	2	0.28
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD11	3	0.28
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD12	3	0.28
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD13	3	0.28
(1,80)	1:33:A:VAL:H	1:68:A:GLN:H	9	0.28
(1,39)	1:31:A:LEU:HD21	1:53:A:PHE:HD1	1	0.28
(1,39)	1:31:A:LEU:HD21	1:53:A:PHE:HD2	1	0.28
(1,39)	1:31:A:LEU:HD22	1:53:A:PHE:HD1	1	0.28
(1,39)	1:31:A:LEU:HD22	1:53:A:PHE:HD2	1	0.28
(1,39)	1:31:A:LEU:HD23	1:53:A:PHE:HD1	1	0.28
(1,39)	1:31:A:LEU:HD23	1:53:A:PHE:HD2	1	0.28
(1,19)	1:30:A:ALA:H	1:133:A:SER:H	9	0.28
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD11	2	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD12	2	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD13	2	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD21	2	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD22	2	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD23	2	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD11	7	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD12	7	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD13	7	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD21	7	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD22	7	0.27
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD23	7	0.27
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG21	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG22	6	0.27
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG23	6	0.27
(1,703)	1:173:A:ASP:H	1:181:A:VAL:HG11	9	0.27
(1,703)	1:173:A:ASP:H	1:181:A:VAL:HG12	9	0.27
(1,703)	1:173:A:ASP:H	1:181:A:VAL:HG13	9	0.27
(1,703)	1:173:A:ASP:H	1:181:A:VAL:HG21	9	0.27
(1,703)	1:173:A:ASP:H	1:181:A:VAL:HG22	9	0.27
(1,703)	1:173:A:ASP:H	1:181:A:VAL:HG23	9	0.27
(1,671)	1:159:A:VAL:HB	1:183:A:SER:H	9	0.27
(1,650)	1:157:A:VAL:H	1:183:A:SER:H	8	0.27
(1,632)	1:156:A:ILE:HD11	1:196:A:ARG:H	1	0.27
(1,632)	1:156:A:ILE:HD12	1:196:A:ARG:H	1	0.27
(1,632)	1:156:A:ILE:HD13	1:196:A:ARG:H	1	0.27
(1,546)	1:141:A:GLY:H	1:157:A:VAL:HG11	3	0.27
(1,546)	1:141:A:GLY:H	1:157:A:VAL:HG12	3	0.27
(1,546)	1:141:A:GLY:H	1:157:A:VAL:HG13	3	0.27
(1,506)	1:136:A:VAL:H	1:148:A:SER:H	5	0.27
(1,444)	1:116:A:VAL:H	1:118:A:GLY:H	4	0.27
(1,439)	1:115:A:LYS:H	1:117:A:ILE:H	10	0.27
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	1	0.27
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG21	1	0.27
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG22	1	0.27
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG23	1	0.27
(1,358)	1:89:A:GLU:H	1:106:A:GLN:H	6	0.27
(1,346)	1:84:A:ARG:H	1:86:A:GLY:H	7	0.27
(1,271)	1:64:A:ARG:H	1:115:A:LYS:H	2	0.27
(1,258)	1:60:A:TYR:H	1:62:A:PHE:HD1	9	0.27
(1,258)	1:60:A:TYR:H	1:62:A:PHE:HD2	9	0.27
(1,184)	1:49:A:LEU:H	1:51:A:ASP:H	4	0.27
(1,109)	1:39:A:VAL:HG11	1:98:A:PHE:HE1	4	0.27
(1,109)	1:39:A:VAL:HG11	1:98:A:PHE:HE2	4	0.27
(1,109)	1:39:A:VAL:HG12	1:98:A:PHE:HE1	4	0.27
(1,109)	1:39:A:VAL:HG12	1:98:A:PHE:HE2	4	0.27
(1,109)	1:39:A:VAL:HG13	1:98:A:PHE:HE1	4	0.27
(1,109)	1:39:A:VAL:HG13	1:98:A:PHE:HE2	4	0.27
(1,80)	1:33:A:VAL:H	1:68:A:GLN:H	3	0.27
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD11	10	0.27
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD12	10	0.27
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD13	10	0.27
(1,46)	1:31:A:LEU:H	1:65:A:LEU:H	2	0.27
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD11	9	0.27
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD12	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD13	9	0.27
(1,17)	1:29:A:LYS:H	1:63:A:VAL:HG11	4	0.27
(1,17)	1:29:A:LYS:H	1:63:A:VAL:HG12	4	0.27
(1,17)	1:29:A:LYS:H	1:63:A:VAL:HG13	4	0.27
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD11	9	0.26
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD12	9	0.26
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD13	9	0.26
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD21	9	0.26
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD22	9	0.26
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD23	9	0.26
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD11	9	0.26
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD12	9	0.26
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD13	9	0.26
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD21	9	0.26
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD22	9	0.26
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD23	9	0.26
(1,668)	1:159:A:VAL:HG11	1:175:A:PHE:H	7	0.26
(1,668)	1:159:A:VAL:HG12	1:175:A:PHE:H	7	0.26
(1,668)	1:159:A:VAL:HG13	1:175:A:PHE:H	7	0.26
(1,668)	1:159:A:VAL:HG21	1:175:A:PHE:H	7	0.26
(1,668)	1:159:A:VAL:HG22	1:175:A:PHE:H	7	0.26
(1,668)	1:159:A:VAL:HG23	1:175:A:PHE:H	7	0.26
(1,568)	1:145:A:ILE:HD11	1:172:A:ALA:H	8	0.26
(1,568)	1:145:A:ILE:HD12	1:172:A:ALA:H	8	0.26
(1,568)	1:145:A:ILE:HD13	1:172:A:ALA:H	8	0.26
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD11	10	0.26
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD12	10	0.26
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD13	10	0.26
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD21	10	0.26
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD22	10	0.26
(1,516)	1:137:A:ILE:HD11	1:191:A:LEU:HD23	10	0.26
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD11	10	0.26
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD12	10	0.26
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD13	10	0.26
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD21	10	0.26
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD22	10	0.26
(1,516)	1:137:A:ILE:HD12	1:191:A:LEU:HD23	10	0.26
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD11	10	0.26
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD12	10	0.26
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD13	10	0.26
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD21	10	0.26
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD22	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:137:A:ILE:HD13	1:191:A:LEU:HD23	10	0.26
(1,450)	1:124:A:LYS:H	1:125:A:MET:H	1	0.26
(1,422)	1:109:A:LEU:HD11	1:115:A:LYS:H	2	0.26
(1,422)	1:109:A:LEU:HD12	1:115:A:LYS:H	2	0.26
(1,422)	1:109:A:LEU:HD13	1:115:A:LYS:H	2	0.26
(1,422)	1:109:A:LEU:HD21	1:115:A:LYS:H	2	0.26
(1,422)	1:109:A:LEU:HD22	1:115:A:LYS:H	2	0.26
(1,422)	1:109:A:LEU:HD23	1:115:A:LYS:H	2	0.26
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG11	5	0.26
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG12	5	0.26
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG13	5	0.26
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD11	6	0.26
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD12	6	0.26
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD13	6	0.26
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD21	6	0.26
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD22	6	0.26
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD23	6	0.26
(1,383)	1:105:A:ARG:H	1:116:A:VAL:HG11	1	0.26
(1,383)	1:105:A:ARG:H	1:116:A:VAL:HG12	1	0.26
(1,383)	1:105:A:ARG:H	1:116:A:VAL:HG13	1	0.26
(1,383)	1:105:A:ARG:H	1:116:A:VAL:HG21	1	0.26
(1,383)	1:105:A:ARG:H	1:116:A:VAL:HG22	1	0.26
(1,383)	1:105:A:ARG:H	1:116:A:VAL:HG23	1	0.26
(1,346)	1:84:A:ARG:H	1:86:A:GLY:H	2	0.26
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG11	1	0.26
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG12	1	0.26
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG13	1	0.26
(1,263)	1:63:A:VAL:H	1:115:A:LYS:H	2	0.26
(1,263)	1:63:A:VAL:H	1:115:A:LYS:H	9	0.26
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	8	0.26
(1,222)	1:55:A:GLN:H	1:57:A:LEU:H	5	0.26
(1,220)	1:54:A:CYS:H	1:58:A:ILE:H	3	0.26
(1,153)	1:47:A:CYS:H	1:52:A:GLU:H	8	0.26
(1,132)	1:44:A:LEU:HD21	1:47:A:CYS:H	1	0.26
(1,132)	1:44:A:LEU:HD22	1:47:A:CYS:H	1	0.26
(1,132)	1:44:A:LEU:HD23	1:47:A:CYS:H	1	0.26
(1,83)	1:34:A:THR:H	1:137:A:ILE:H	7	0.26
(1,53)	1:32:A:PHE:HD1	1:136:A:VAL:H	3	0.26
(1,53)	1:32:A:PHE:HD2	1:136:A:VAL:H	3	0.26
(1,39)	1:31:A:LEU:HD21	1:53:A:PHE:HD1	10	0.26
(1,39)	1:31:A:LEU:HD21	1:53:A:PHE:HD2	10	0.26
(1,39)	1:31:A:LEU:HD22	1:53:A:PHE:HD1	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:31:A:LEU:HD22	1:53:A:PHE:HD2	10	0.26
(1,39)	1:31:A:LEU:HD23	1:53:A:PHE:HD1	10	0.26
(1,39)	1:31:A:LEU:HD23	1:53:A:PHE:HD2	10	0.26
(1,29)	1:31:A:LEU:HD11	1:134:A:ASP:H	2	0.26
(1,29)	1:31:A:LEU:HD12	1:134:A:ASP:H	2	0.26
(1,29)	1:31:A:LEU:HD13	1:134:A:ASP:H	2	0.26
(1,29)	1:31:A:LEU:HD21	1:134:A:ASP:H	2	0.26
(1,29)	1:31:A:LEU:HD22	1:134:A:ASP:H	2	0.26
(1,29)	1:31:A:LEU:HD23	1:134:A:ASP:H	2	0.26
(1,14)	1:28:A:GLU:H	1:30:A:ALA:H	7	0.26
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD11	8	0.25
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD12	8	0.25
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD13	8	0.25
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD21	8	0.25
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD22	8	0.25
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD23	8	0.25
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	6	0.25
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	6	0.25
(1,761)	1:181:A:VAL:H	1:183:A:SER:H	8	0.25
(1,749)	1:180:A:TYR:H	1:181:A:VAL:H	2	0.25
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD11	9	0.25
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD12	9	0.25
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD13	9	0.25
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD21	9	0.25
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD22	9	0.25
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD23	9	0.25
(1,588)	1:148:A:SER:H	1:155:A:LEU:HD11	6	0.25
(1,588)	1:148:A:SER:H	1:155:A:LEU:HD12	6	0.25
(1,588)	1:148:A:SER:H	1:155:A:LEU:HD13	6	0.25
(1,588)	1:148:A:SER:H	1:155:A:LEU:HD21	6	0.25
(1,588)	1:148:A:SER:H	1:155:A:LEU:HD22	6	0.25
(1,588)	1:148:A:SER:H	1:155:A:LEU:HD23	6	0.25
(1,568)	1:145:A:ILE:HD11	1:172:A:ALA:H	9	0.25
(1,568)	1:145:A:ILE:HD12	1:172:A:ALA:H	9	0.25
(1,568)	1:145:A:ILE:HD13	1:172:A:ALA:H	9	0.25
(1,409)	1:108:A:VAL:HG11	1:113:A:LYS:H	2	0.25
(1,409)	1:108:A:VAL:HG12	1:113:A:LYS:H	2	0.25
(1,409)	1:108:A:VAL:HG13	1:113:A:LYS:H	2	0.25
(1,409)	1:108:A:VAL:HG21	1:113:A:LYS:H	2	0.25
(1,409)	1:108:A:VAL:HG22	1:113:A:LYS:H	2	0.25
(1,409)	1:108:A:VAL:HG23	1:113:A:LYS:H	2	0.25
(1,405)	1:108:A:VAL:H	1:110:A:MET:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD11	2	0.25
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD12	2	0.25
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD13	2	0.25
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	7	0.25
(1,263)	1:63:A:VAL:H	1:115:A:LYS:H	5	0.25
(1,262)	1:63:A:VAL:HG11	1:115:A:LYS:H	1	0.25
(1,262)	1:63:A:VAL:HG12	1:115:A:LYS:H	1	0.25
(1,262)	1:63:A:VAL:HG13	1:115:A:LYS:H	1	0.25
(1,262)	1:63:A:VAL:HG21	1:115:A:LYS:H	1	0.25
(1,262)	1:63:A:VAL:HG22	1:115:A:LYS:H	1	0.25
(1,262)	1:63:A:VAL:HG23	1:115:A:LYS:H	1	0.25
(1,184)	1:49:A:LEU:H	1:51:A:ASP:H	3	0.25
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD11	10	0.25
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD12	10	0.25
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD13	10	0.25
(1,29)	1:31:A:LEU:HD11	1:134:A:ASP:H	4	0.25
(1,29)	1:31:A:LEU:HD12	1:134:A:ASP:H	4	0.25
(1,29)	1:31:A:LEU:HD13	1:134:A:ASP:H	4	0.25
(1,29)	1:31:A:LEU:HD21	1:134:A:ASP:H	4	0.25
(1,29)	1:31:A:LEU:HD22	1:134:A:ASP:H	4	0.25
(1,29)	1:31:A:LEU:HD23	1:134:A:ASP:H	4	0.25
(1,867)	1:203:A:LEU:HD11	1:208:A:VAL:H	10	0.24
(1,867)	1:203:A:LEU:HD12	1:208:A:VAL:H	10	0.24
(1,867)	1:203:A:LEU:HD13	1:208:A:VAL:H	10	0.24
(1,867)	1:203:A:LEU:HD21	1:208:A:VAL:H	10	0.24
(1,867)	1:203:A:LEU:HD22	1:208:A:VAL:H	10	0.24
(1,867)	1:203:A:LEU:HD23	1:208:A:VAL:H	10	0.24
(1,765)	1:182:A:TRP:HE1	1:197:A:ALA:H	1	0.24
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG21	5	0.24
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG22	5	0.24
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG23	5	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD11	3	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD12	3	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD13	3	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD21	3	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD22	3	0.24
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD23	3	0.24
(1,660)	1:159:A:VAL:HG11	1:169:A:GLN:H	2	0.24
(1,660)	1:159:A:VAL:HG12	1:169:A:GLN:H	2	0.24
(1,660)	1:159:A:VAL:HG13	1:169:A:GLN:H	2	0.24
(1,660)	1:159:A:VAL:HG21	1:169:A:GLN:H	2	0.24
(1,660)	1:159:A:VAL:HG22	1:169:A:GLN:H	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:159:A:VAL:HG23	1:169:A:GLN:H	2	0.24
(1,596)	1:149:A:LEU:HD11	1:153:A:LYS:H	5	0.24
(1,596)	1:149:A:LEU:HD12	1:153:A:LYS:H	5	0.24
(1,596)	1:149:A:LEU:HD13	1:153:A:LYS:H	5	0.24
(1,596)	1:149:A:LEU:HD21	1:153:A:LYS:H	5	0.24
(1,596)	1:149:A:LEU:HD22	1:153:A:LYS:H	5	0.24
(1,596)	1:149:A:LEU:HD23	1:153:A:LYS:H	5	0.24
(1,567)	1:145:A:ILE:HD11	1:171:A:ILE:H	3	0.24
(1,567)	1:145:A:ILE:HD12	1:171:A:ILE:H	3	0.24
(1,567)	1:145:A:ILE:HD13	1:171:A:ILE:H	3	0.24
(1,543)	1:140:A:ALA:HB1	1:160:A:ASN:H	4	0.24
(1,543)	1:140:A:ALA:HB2	1:160:A:ASN:H	4	0.24
(1,543)	1:140:A:ALA:HB3	1:160:A:ASN:H	4	0.24
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG11	4	0.24
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG12	4	0.24
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG13	4	0.24
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG21	4	0.24
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG22	4	0.24
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG23	4	0.24
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG11	4	0.24
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG12	4	0.24
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG13	4	0.24
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG21	4	0.24
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG22	4	0.24
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG23	4	0.24
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG11	4	0.24
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG12	4	0.24
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG13	4	0.24
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG21	4	0.24
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG22	4	0.24
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG23	4	0.24
(1,526)	1:138:A:SER:H	1:157:A:VAL:H	1	0.24
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG11	9	0.24
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG12	9	0.24
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG13	9	0.24
(1,363)	1:93:A:ILE:HD11	1:96:A:ASP:H	10	0.24
(1,363)	1:93:A:ILE:HD12	1:96:A:ASP:H	10	0.24
(1,363)	1:93:A:ILE:HD13	1:96:A:ASP:H	10	0.24
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG11	7	0.24
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG12	7	0.24
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG13	7	0.24
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG11	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG12	10	0.24
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG13	10	0.24
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG11	10	0.24
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG12	10	0.24
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG13	10	0.24
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG21	10	0.24
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG22	10	0.24
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG23	10	0.24
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG11	10	0.24
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG12	10	0.24
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG13	10	0.24
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG21	10	0.24
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG22	10	0.24
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG23	10	0.24
(1,262)	1:63:A:VAL:HG11	1:115:A:LYS:H	8	0.24
(1,262)	1:63:A:VAL:HG12	1:115:A:LYS:H	8	0.24
(1,262)	1:63:A:VAL:HG13	1:115:A:LYS:H	8	0.24
(1,262)	1:63:A:VAL:HG21	1:115:A:LYS:H	8	0.24
(1,262)	1:63:A:VAL:HG22	1:115:A:LYS:H	8	0.24
(1,262)	1:63:A:VAL:HG23	1:115:A:LYS:H	8	0.24
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	4	0.24
(1,164)	1:48:A:VAL:HG11	1:53:A:PHE:H	4	0.24
(1,164)	1:48:A:VAL:HG12	1:53:A:PHE:H	4	0.24
(1,164)	1:48:A:VAL:HG13	1:53:A:PHE:H	4	0.24
(1,164)	1:48:A:VAL:HG21	1:53:A:PHE:H	4	0.24
(1,164)	1:48:A:VAL:HG22	1:53:A:PHE:H	4	0.24
(1,164)	1:48:A:VAL:HG23	1:53:A:PHE:H	4	0.24
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD11	9	0.24
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD12	9	0.24
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD13	9	0.24
(1,101)	1:39:A:VAL:HG11	1:44:A:LEU:H	6	0.24
(1,101)	1:39:A:VAL:HG12	1:44:A:LEU:H	6	0.24
(1,101)	1:39:A:VAL:HG13	1:44:A:LEU:H	6	0.24
(1,101)	1:39:A:VAL:HG21	1:44:A:LEU:H	6	0.24
(1,101)	1:39:A:VAL:HG22	1:44:A:LEU:H	6	0.24
(1,101)	1:39:A:VAL:HG23	1:44:A:LEU:H	6	0.24
(1,35)	1:31:A:LEU:HD11	1:32:A:PHE:H	7	0.24
(1,35)	1:31:A:LEU:HD12	1:32:A:PHE:H	7	0.24
(1,35)	1:31:A:LEU:HD13	1:32:A:PHE:H	7	0.24
(1,35)	1:31:A:LEU:HD21	1:32:A:PHE:H	7	0.24
(1,35)	1:31:A:LEU:HD22	1:32:A:PHE:H	7	0.24
(1,35)	1:31:A:LEU:HD23	1:32:A:PHE:H	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:30:A:ALA:H	1:135:A:LEU:H	7	0.24
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE1	6	0.24
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE2	6	0.24
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE1	6	0.24
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE2	6	0.24
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE1	6	0.24
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE2	6	0.24
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	9	0.23
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	9	0.23
(1,821)	1:191:A:LEU:HD21	1:194:A:GLY:H	1	0.23
(1,821)	1:191:A:LEU:HD22	1:194:A:GLY:H	1	0.23
(1,821)	1:191:A:LEU:HD23	1:194:A:GLY:H	1	0.23
(1,778)	1:184:A:CYS:H	1:184:A:CYS:HG	4	0.23
(1,686)	1:168:A:GLN:H	1:171:A:ILE:H	2	0.23
(1,660)	1:159:A:VAL:HG11	1:169:A:GLN:H	5	0.23
(1,660)	1:159:A:VAL:HG12	1:169:A:GLN:H	5	0.23
(1,660)	1:159:A:VAL:HG13	1:169:A:GLN:H	5	0.23
(1,660)	1:159:A:VAL:HG21	1:169:A:GLN:H	5	0.23
(1,660)	1:159:A:VAL:HG22	1:169:A:GLN:H	5	0.23
(1,660)	1:159:A:VAL:HG23	1:169:A:GLN:H	5	0.23
(1,597)	1:149:A:LEU:H	1:153:A:LYS:H	9	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG11	5	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG12	5	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG13	5	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG21	5	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG22	5	0.23
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG23	5	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG11	5	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG12	5	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG13	5	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG21	5	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG22	5	0.23
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG23	5	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG11	5	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG12	5	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG13	5	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG21	5	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG22	5	0.23
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG23	5	0.23
(1,537)	1:140:A:ALA:H	1:141:A:GLY:H	1	0.23
(1,506)	1:136:A:VAL:H	1:148:A:SER:H	2	0.23
(1,447)	1:117:A:ILE:HD11	1:118:A:GLY:H	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,447)	1:117:A:ILE:HD12	1:118:A:GLY:H	8	0.23
(1,447)	1:117:A:ILE:HD13	1:118:A:GLY:H	8	0.23
(1,400)	1:108:A:VAL:H	1:108:A:VAL:HG21	8	0.23
(1,400)	1:108:A:VAL:H	1:108:A:VAL:HG22	8	0.23
(1,400)	1:108:A:VAL:H	1:108:A:VAL:HG23	8	0.23
(1,376)	1:100:A:CYS:H	1:101:A:GLY:H	8	0.23
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG21	8	0.23
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG22	8	0.23
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG23	8	0.23
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG11	5	0.23
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG12	5	0.23
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG13	5	0.23
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG21	5	0.23
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG22	5	0.23
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG23	5	0.23
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG11	5	0.23
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG12	5	0.23
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG13	5	0.23
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG21	5	0.23
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG22	5	0.23
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG23	5	0.23
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG11	5	0.23
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG12	5	0.23
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG13	5	0.23
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG21	5	0.23
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG22	5	0.23
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG23	5	0.23
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG11	5	0.23
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG12	5	0.23
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG13	5	0.23
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG21	5	0.23
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG22	5	0.23
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG23	5	0.23
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG11	5	0.23
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG12	5	0.23
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG13	5	0.23
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG21	5	0.23
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG22	5	0.23
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG23	5	0.23
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG11	5	0.23
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG12	5	0.23
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG13	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG21	5	0.23
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG22	5	0.23
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG23	5	0.23
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	6	0.23
(1,164)	1:48:A:VAL:HG11	1:53:A:PHE:H	5	0.23
(1,164)	1:48:A:VAL:HG12	1:53:A:PHE:H	5	0.23
(1,164)	1:48:A:VAL:HG13	1:53:A:PHE:H	5	0.23
(1,164)	1:48:A:VAL:HG21	1:53:A:PHE:H	5	0.23
(1,164)	1:48:A:VAL:HG22	1:53:A:PHE:H	5	0.23
(1,164)	1:48:A:VAL:HG23	1:53:A:PHE:H	5	0.23
(1,53)	1:32:A:PHE:HD1	1:136:A:VAL:H	7	0.23
(1,53)	1:32:A:PHE:HD2	1:136:A:VAL:H	7	0.23
(1,39)	1:31:A:LEU:HD21	1:53:A:PHE:HD1	4	0.23
(1,39)	1:31:A:LEU:HD21	1:53:A:PHE:HD2	4	0.23
(1,39)	1:31:A:LEU:HD22	1:53:A:PHE:HD1	4	0.23
(1,39)	1:31:A:LEU:HD22	1:53:A:PHE:HD2	4	0.23
(1,39)	1:31:A:LEU:HD23	1:53:A:PHE:HD1	4	0.23
(1,39)	1:31:A:LEU:HD23	1:53:A:PHE:HD2	4	0.23
(1,17)	1:29:A:LYS:H	1:63:A:VAL:HG11	7	0.23
(1,17)	1:29:A:LYS:H	1:63:A:VAL:HG12	7	0.23
(1,17)	1:29:A:LYS:H	1:63:A:VAL:HG13	7	0.23
(1,765)	1:182:A:TRP:HE1	1:197:A:ALA:H	8	0.22
(1,674)	1:159:A:VAL:HG11	1:185:A:ALA:HB1	3	0.22
(1,674)	1:159:A:VAL:HG11	1:185:A:ALA:HB2	3	0.22
(1,674)	1:159:A:VAL:HG11	1:185:A:ALA:HB3	3	0.22
(1,674)	1:159:A:VAL:HG12	1:185:A:ALA:HB1	3	0.22
(1,674)	1:159:A:VAL:HG12	1:185:A:ALA:HB2	3	0.22
(1,674)	1:159:A:VAL:HG12	1:185:A:ALA:HB3	3	0.22
(1,674)	1:159:A:VAL:HG13	1:185:A:ALA:HB1	3	0.22
(1,674)	1:159:A:VAL:HG13	1:185:A:ALA:HB2	3	0.22
(1,674)	1:159:A:VAL:HG13	1:185:A:ALA:HB3	3	0.22
(1,674)	1:159:A:VAL:HG21	1:185:A:ALA:HB1	3	0.22
(1,674)	1:159:A:VAL:HG21	1:185:A:ALA:HB2	3	0.22
(1,674)	1:159:A:VAL:HG21	1:185:A:ALA:HB3	3	0.22
(1,674)	1:159:A:VAL:HG22	1:185:A:ALA:HB1	3	0.22
(1,674)	1:159:A:VAL:HG22	1:185:A:ALA:HB2	3	0.22
(1,674)	1:159:A:VAL:HG22	1:185:A:ALA:HB3	3	0.22
(1,674)	1:159:A:VAL:HG23	1:185:A:ALA:HB1	3	0.22
(1,674)	1:159:A:VAL:HG23	1:185:A:ALA:HB2	3	0.22
(1,674)	1:159:A:VAL:HG23	1:185:A:ALA:HB3	3	0.22
(1,670)	1:159:A:VAL:HG11	1:181:A:VAL:H	5	0.22
(1,670)	1:159:A:VAL:HG12	1:181:A:VAL:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:159:A:VAL:HG13	1:181:A:VAL:H	5	0.22
(1,670)	1:159:A:VAL:HG21	1:181:A:VAL:H	5	0.22
(1,670)	1:159:A:VAL:HG22	1:181:A:VAL:H	5	0.22
(1,670)	1:159:A:VAL:HG23	1:181:A:VAL:H	5	0.22
(1,663)	1:159:A:VAL:HG11	1:172:A:ALA:H	1	0.22
(1,663)	1:159:A:VAL:HG12	1:172:A:ALA:H	1	0.22
(1,663)	1:159:A:VAL:HG13	1:172:A:ALA:H	1	0.22
(1,620)	1:155:A:LEU:HD11	1:156:A:ILE:HD11	8	0.22
(1,620)	1:155:A:LEU:HD11	1:156:A:ILE:HD12	8	0.22
(1,620)	1:155:A:LEU:HD11	1:156:A:ILE:HD13	8	0.22
(1,620)	1:155:A:LEU:HD12	1:156:A:ILE:HD11	8	0.22
(1,620)	1:155:A:LEU:HD12	1:156:A:ILE:HD12	8	0.22
(1,620)	1:155:A:LEU:HD12	1:156:A:ILE:HD13	8	0.22
(1,620)	1:155:A:LEU:HD13	1:156:A:ILE:HD11	8	0.22
(1,620)	1:155:A:LEU:HD13	1:156:A:ILE:HD12	8	0.22
(1,620)	1:155:A:LEU:HD13	1:156:A:ILE:HD13	8	0.22
(1,620)	1:155:A:LEU:HD21	1:156:A:ILE:HD11	8	0.22
(1,620)	1:155:A:LEU:HD21	1:156:A:ILE:HD12	8	0.22
(1,620)	1:155:A:LEU:HD21	1:156:A:ILE:HD13	8	0.22
(1,620)	1:155:A:LEU:HD22	1:156:A:ILE:HD11	8	0.22
(1,620)	1:155:A:LEU:HD22	1:156:A:ILE:HD12	8	0.22
(1,620)	1:155:A:LEU:HD22	1:156:A:ILE:HD13	8	0.22
(1,620)	1:155:A:LEU:HD23	1:156:A:ILE:HD11	8	0.22
(1,620)	1:155:A:LEU:HD23	1:156:A:ILE:HD12	8	0.22
(1,620)	1:155:A:LEU:HD23	1:156:A:ILE:HD13	8	0.22
(1,610)	1:150:A:ARG:H	1:153:A:LYS:H	4	0.22
(1,610)	1:150:A:ARG:H	1:153:A:LYS:H	6	0.22
(1,529)	1:139:A:HIS:H	1:140:A:ALA:H	7	0.22
(1,494)	1:135:A:LEU:H	1:137:A:ILE:H	4	0.22
(1,410)	1:108:A:VAL:HG11	1:114:A:LEU:H	3	0.22
(1,410)	1:108:A:VAL:HG12	1:114:A:LEU:H	3	0.22
(1,410)	1:108:A:VAL:HG13	1:114:A:LEU:H	3	0.22
(1,410)	1:108:A:VAL:HG21	1:114:A:LEU:H	3	0.22
(1,410)	1:108:A:VAL:HG22	1:114:A:LEU:H	3	0.22
(1,410)	1:108:A:VAL:HG23	1:114:A:LEU:H	3	0.22
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG11	4	0.22
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG12	4	0.22
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG13	4	0.22
(1,389)	1:106:A:GLN:H	1:118:A:GLY:H	3	0.22
(1,380)	1:104:A:ALA:H	1:118:A:GLY:H	1	0.22
(1,359)	1:89:A:GLU:H	1:107:A:TYR:H	1	0.22
(1,359)	1:89:A:GLU:H	1:107:A:TYR:H	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:81:A:VAL:HG11	1:118:A:GLY:H	1	0.22
(1,326)	1:81:A:VAL:HG12	1:118:A:GLY:H	1	0.22
(1,326)	1:81:A:VAL:HG13	1:118:A:GLY:H	1	0.22
(1,326)	1:81:A:VAL:HG21	1:118:A:GLY:H	1	0.22
(1,326)	1:81:A:VAL:HG22	1:118:A:GLY:H	1	0.22
(1,326)	1:81:A:VAL:HG23	1:118:A:GLY:H	1	0.22
(1,220)	1:54:A:CYS:H	1:58:A:ILE:H	6	0.22
(1,195)	1:49:A:LEU:HD11	1:81:A:VAL:HG11	2	0.22
(1,195)	1:49:A:LEU:HD11	1:81:A:VAL:HG12	2	0.22
(1,195)	1:49:A:LEU:HD11	1:81:A:VAL:HG13	2	0.22
(1,195)	1:49:A:LEU:HD11	1:81:A:VAL:HG21	2	0.22
(1,195)	1:49:A:LEU:HD11	1:81:A:VAL:HG22	2	0.22
(1,195)	1:49:A:LEU:HD11	1:81:A:VAL:HG23	2	0.22
(1,195)	1:49:A:LEU:HD12	1:81:A:VAL:HG11	2	0.22
(1,195)	1:49:A:LEU:HD12	1:81:A:VAL:HG12	2	0.22
(1,195)	1:49:A:LEU:HD12	1:81:A:VAL:HG13	2	0.22
(1,195)	1:49:A:LEU:HD12	1:81:A:VAL:HG21	2	0.22
(1,195)	1:49:A:LEU:HD12	1:81:A:VAL:HG22	2	0.22
(1,195)	1:49:A:LEU:HD12	1:81:A:VAL:HG23	2	0.22
(1,195)	1:49:A:LEU:HD13	1:81:A:VAL:HG11	2	0.22
(1,195)	1:49:A:LEU:HD13	1:81:A:VAL:HG12	2	0.22
(1,195)	1:49:A:LEU:HD13	1:81:A:VAL:HG13	2	0.22
(1,195)	1:49:A:LEU:HD13	1:81:A:VAL:HG21	2	0.22
(1,195)	1:49:A:LEU:HD13	1:81:A:VAL:HG22	2	0.22
(1,195)	1:49:A:LEU:HD13	1:81:A:VAL:HG23	2	0.22
(1,195)	1:49:A:LEU:HD21	1:81:A:VAL:HG11	2	0.22
(1,195)	1:49:A:LEU:HD21	1:81:A:VAL:HG12	2	0.22
(1,195)	1:49:A:LEU:HD21	1:81:A:VAL:HG13	2	0.22
(1,195)	1:49:A:LEU:HD21	1:81:A:VAL:HG21	2	0.22
(1,195)	1:49:A:LEU:HD21	1:81:A:VAL:HG22	2	0.22
(1,195)	1:49:A:LEU:HD21	1:81:A:VAL:HG23	2	0.22
(1,195)	1:49:A:LEU:HD22	1:81:A:VAL:HG11	2	0.22
(1,195)	1:49:A:LEU:HD22	1:81:A:VAL:HG12	2	0.22
(1,195)	1:49:A:LEU:HD22	1:81:A:VAL:HG13	2	0.22
(1,195)	1:49:A:LEU:HD22	1:81:A:VAL:HG21	2	0.22
(1,195)	1:49:A:LEU:HD22	1:81:A:VAL:HG22	2	0.22
(1,195)	1:49:A:LEU:HD22	1:81:A:VAL:HG23	2	0.22
(1,195)	1:49:A:LEU:HD23	1:81:A:VAL:HG11	2	0.22
(1,195)	1:49:A:LEU:HD23	1:81:A:VAL:HG12	2	0.22
(1,195)	1:49:A:LEU:HD23	1:81:A:VAL:HG13	2	0.22
(1,195)	1:49:A:LEU:HD23	1:81:A:VAL:HG21	2	0.22
(1,195)	1:49:A:LEU:HD23	1:81:A:VAL:HG22	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:49:A:LEU:HD23	1:81:A:VAL:HG23	2	0.22
(1,190)	1:49:A:LEU:HD11	1:77:A:PHE:HD1	6	0.22
(1,190)	1:49:A:LEU:HD11	1:77:A:PHE:HD2	6	0.22
(1,190)	1:49:A:LEU:HD12	1:77:A:PHE:HD1	6	0.22
(1,190)	1:49:A:LEU:HD12	1:77:A:PHE:HD2	6	0.22
(1,190)	1:49:A:LEU:HD13	1:77:A:PHE:HD1	6	0.22
(1,190)	1:49:A:LEU:HD13	1:77:A:PHE:HD2	6	0.22
(1,187)	1:49:A:LEU:HD11	1:65:A:LEU:H	10	0.22
(1,187)	1:49:A:LEU:HD12	1:65:A:LEU:H	10	0.22
(1,187)	1:49:A:LEU:HD13	1:65:A:LEU:H	10	0.22
(1,187)	1:49:A:LEU:HD21	1:65:A:LEU:H	10	0.22
(1,187)	1:49:A:LEU:HD22	1:65:A:LEU:H	10	0.22
(1,187)	1:49:A:LEU:HD23	1:65:A:LEU:H	10	0.22
(1,168)	1:49:A:LEU:HD11	1:107:A:TYR:H	8	0.22
(1,168)	1:49:A:LEU:HD12	1:107:A:TYR:H	8	0.22
(1,168)	1:49:A:LEU:HD13	1:107:A:TYR:H	8	0.22
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	5	0.22
(1,132)	1:44:A:LEU:HD21	1:47:A:CYS:H	9	0.22
(1,132)	1:44:A:LEU:HD22	1:47:A:CYS:H	9	0.22
(1,132)	1:44:A:LEU:HD23	1:47:A:CYS:H	9	0.22
(1,110)	1:39:A:VAL:HG21	1:98:A:PHE:HE1	7	0.22
(1,110)	1:39:A:VAL:HG21	1:98:A:PHE:HE2	7	0.22
(1,110)	1:39:A:VAL:HG22	1:98:A:PHE:HE1	7	0.22
(1,110)	1:39:A:VAL:HG22	1:98:A:PHE:HE2	7	0.22
(1,110)	1:39:A:VAL:HG23	1:98:A:PHE:HE1	7	0.22
(1,110)	1:39:A:VAL:HG23	1:98:A:PHE:HE2	7	0.22
(1,83)	1:34:A:THR:H	1:137:A:ILE:H	3	0.22
(1,52)	1:32:A:PHE:H	1:135:A:LEU:H	6	0.22
(1,31)	1:31:A:LEU:H	1:135:A:LEU:H	7	0.22
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD11	3	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD12	3	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD13	3	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD21	3	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD22	3	0.21
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD23	3	0.21
(1,841)	1:195:A:LEU:HD11	1:199:A:GLN:H	1	0.21
(1,841)	1:195:A:LEU:HD12	1:199:A:GLN:H	1	0.21
(1,841)	1:195:A:LEU:HD13	1:199:A:GLN:H	1	0.21
(1,841)	1:195:A:LEU:HD21	1:199:A:GLN:H	1	0.21
(1,841)	1:195:A:LEU:HD22	1:199:A:GLN:H	1	0.21
(1,841)	1:195:A:LEU:HD23	1:199:A:GLN:H	1	0.21
(1,841)	1:195:A:LEU:HD11	1:199:A:GLN:H	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	1:195:A:LEU:HD12	1:199:A:GLN:H	6	0.21
(1,841)	1:195:A:LEU:HD13	1:199:A:GLN:H	6	0.21
(1,841)	1:195:A:LEU:HD21	1:199:A:GLN:H	6	0.21
(1,841)	1:195:A:LEU:HD22	1:199:A:GLN:H	6	0.21
(1,841)	1:195:A:LEU:HD23	1:199:A:GLN:H	6	0.21
(1,741)	1:178:A:LEU:HD11	1:180:A:TYR:H	1	0.21
(1,741)	1:178:A:LEU:HD12	1:180:A:TYR:H	1	0.21
(1,741)	1:178:A:LEU:HD13	1:180:A:TYR:H	1	0.21
(1,741)	1:178:A:LEU:HD21	1:180:A:TYR:H	1	0.21
(1,741)	1:178:A:LEU:HD22	1:180:A:TYR:H	1	0.21
(1,741)	1:178:A:LEU:HD23	1:180:A:TYR:H	1	0.21
(1,724)	1:176:A:VAL:H	1:180:A:TYR:H	3	0.21
(1,690)	1:170:A:GLN:H	1:173:A:ASP:H	10	0.21
(1,671)	1:159:A:VAL:HB	1:183:A:SER:H	3	0.21
(1,650)	1:157:A:VAL:H	1:183:A:SER:H	10	0.21
(1,632)	1:156:A:ILE:HD11	1:196:A:ARG:H	2	0.21
(1,632)	1:156:A:ILE:HD12	1:196:A:ARG:H	2	0.21
(1,632)	1:156:A:ILE:HD13	1:196:A:ARG:H	2	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD11	6	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD12	6	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD13	6	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD21	6	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD22	6	0.21
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD23	6	0.21
(1,457)	1:126:A:GLN:H	1:129:A:ILE:H	2	0.21
(1,447)	1:117:A:ILE:HD11	1:118:A:GLY:H	6	0.21
(1,447)	1:117:A:ILE:HD12	1:118:A:GLY:H	6	0.21
(1,447)	1:117:A:ILE:HD13	1:118:A:GLY:H	6	0.21
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG11	10	0.21
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG12	10	0.21
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG13	10	0.21
(1,387)	1:106:A:GLN:H	1:117:A:ILE:H	5	0.21
(1,380)	1:104:A:ALA:H	1:118:A:GLY:H	8	0.21
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD11	10	0.21
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD12	10	0.21
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD13	10	0.21
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD21	10	0.21
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD22	10	0.21
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD23	10	0.21
(1,270)	1:63:A:VAL:H	1:65:A:LEU:H	9	0.21
(1,225)	1:55:A:GLN:H	1:58:A:ILE:H	9	0.21
(1,204)	1:51:A:ASP:H	1:54:A:CYS:H	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,193)	1:49:A:LEU:HD11	1:80:A:LEU:H	5	0.21
(1,193)	1:49:A:LEU:HD12	1:80:A:LEU:H	5	0.21
(1,193)	1:49:A:LEU:HD13	1:80:A:LEU:H	5	0.21
(1,193)	1:49:A:LEU:HD21	1:80:A:LEU:H	5	0.21
(1,193)	1:49:A:LEU:HD22	1:80:A:LEU:H	5	0.21
(1,193)	1:49:A:LEU:HD23	1:80:A:LEU:H	5	0.21
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG11	2	0.21
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG12	2	0.21
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG13	2	0.21
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG21	2	0.21
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG22	2	0.21
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG23	2	0.21
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG11	2	0.21
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG12	2	0.21
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG13	2	0.21
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG21	2	0.21
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG22	2	0.21
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG23	2	0.21
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG11	2	0.21
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG12	2	0.21
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG13	2	0.21
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG21	2	0.21
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG22	2	0.21
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG23	2	0.21
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG11	2	0.21
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG12	2	0.21
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG13	2	0.21
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG21	2	0.21
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG22	2	0.21
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG23	2	0.21
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG11	2	0.21
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG12	2	0.21
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG13	2	0.21
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG21	2	0.21
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG22	2	0.21
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG23	2	0.21
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG11	2	0.21
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG12	2	0.21
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG13	2	0.21
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG21	2	0.21
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG22	2	0.21
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG23	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG11	7	0.21
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG12	7	0.21
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG13	7	0.21
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG21	7	0.21
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG22	7	0.21
(1,81)	1:34:A:THR:H	1:136:A:VAL:HG23	7	0.21
(1,890)	1:218:A:LEU:H	1:220:A:GLU:H	1	0.2
(1,761)	1:181:A:VAL:H	1:183:A:SER:H	5	0.2
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG21	4	0.2
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG22	4	0.2
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG23	4	0.2
(1,666)	1:159:A:VAL:HG11	1:173:A:ASP:H	9	0.2
(1,666)	1:159:A:VAL:HG12	1:173:A:ASP:H	9	0.2
(1,666)	1:159:A:VAL:HG13	1:173:A:ASP:H	9	0.2
(1,666)	1:159:A:VAL:HG21	1:173:A:ASP:H	9	0.2
(1,666)	1:159:A:VAL:HG22	1:173:A:ASP:H	9	0.2
(1,666)	1:159:A:VAL:HG23	1:173:A:ASP:H	9	0.2
(1,645)	1:157:A:VAL:H	1:159:A:VAL:HB	7	0.2
(1,470)	1:129:A:ILE:HG21	1:131:A:ASP:H	4	0.2
(1,470)	1:129:A:ILE:HG22	1:131:A:ASP:H	4	0.2
(1,470)	1:129:A:ILE:HG23	1:131:A:ASP:H	4	0.2
(1,370)	1:96:A:ASP:H	1:99:A:GLY:H	5	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD11	6	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD12	6	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD13	6	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD21	6	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD22	6	0.2
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD23	6	0.2
(1,321)	1:81:A:VAL:HG21	1:116:A:VAL:HG21	9	0.2
(1,321)	1:81:A:VAL:HG21	1:116:A:VAL:HG22	9	0.2
(1,321)	1:81:A:VAL:HG21	1:116:A:VAL:HG23	9	0.2
(1,321)	1:81:A:VAL:HG22	1:116:A:VAL:HG21	9	0.2
(1,321)	1:81:A:VAL:HG22	1:116:A:VAL:HG22	9	0.2
(1,321)	1:81:A:VAL:HG22	1:116:A:VAL:HG23	9	0.2
(1,321)	1:81:A:VAL:HG23	1:116:A:VAL:HG21	9	0.2
(1,321)	1:81:A:VAL:HG23	1:116:A:VAL:HG22	9	0.2
(1,321)	1:81:A:VAL:HG23	1:116:A:VAL:HG23	9	0.2
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	9	0.2
(1,225)	1:55:A:GLN:H	1:58:A:ILE:H	2	0.2
(1,204)	1:51:A:ASP:H	1:54:A:CYS:H	7	0.2
(1,203)	1:51:A:ASP:H	1:53:A:PHE:H	5	0.2
(1,31)	1:31:A:LEU:H	1:135:A:LEU:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG11	2	0.2
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG12	2	0.2
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG13	2	0.2
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG21	2	0.2
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG22	2	0.2
(1,15)	1:28:A:GLU:H	1:63:A:VAL:HG23	2	0.2
(1,871)	1:208:A:VAL:HG11	1:211:A:ASN:HD21	3	0.19
(1,871)	1:208:A:VAL:HG11	1:211:A:ASN:HD22	3	0.19
(1,871)	1:208:A:VAL:HG12	1:211:A:ASN:HD21	3	0.19
(1,871)	1:208:A:VAL:HG12	1:211:A:ASN:HD22	3	0.19
(1,871)	1:208:A:VAL:HG13	1:211:A:ASN:HD21	3	0.19
(1,871)	1:208:A:VAL:HG13	1:211:A:ASN:HD22	3	0.19
(1,871)	1:208:A:VAL:HG21	1:211:A:ASN:HD21	3	0.19
(1,871)	1:208:A:VAL:HG21	1:211:A:ASN:HD22	3	0.19
(1,871)	1:208:A:VAL:HG22	1:211:A:ASN:HD21	3	0.19
(1,871)	1:208:A:VAL:HG22	1:211:A:ASN:HD22	3	0.19
(1,871)	1:208:A:VAL:HG23	1:211:A:ASN:HD21	3	0.19
(1,871)	1:208:A:VAL:HG23	1:211:A:ASN:HD22	3	0.19
(1,802)	1:188:A:GLU:H	1:192:A:ILE:HD11	7	0.19
(1,802)	1:188:A:GLU:H	1:192:A:ILE:HD12	7	0.19
(1,802)	1:188:A:GLU:H	1:192:A:ILE:HD13	7	0.19
(1,794)	1:187:A:THR:H	1:189:A:THR:H	5	0.19
(1,734)	1:177:A:GLU:H	1:181:A:VAL:H	5	0.19
(1,668)	1:159:A:VAL:HG11	1:175:A:PHE:H	1	0.19
(1,668)	1:159:A:VAL:HG12	1:175:A:PHE:H	1	0.19
(1,668)	1:159:A:VAL:HG13	1:175:A:PHE:H	1	0.19
(1,668)	1:159:A:VAL:HG21	1:175:A:PHE:H	1	0.19
(1,668)	1:159:A:VAL:HG22	1:175:A:PHE:H	1	0.19
(1,668)	1:159:A:VAL:HG23	1:175:A:PHE:H	1	0.19
(1,567)	1:145:A:ILE:HD11	1:171:A:ILE:H	4	0.19
(1,567)	1:145:A:ILE:HD12	1:171:A:ILE:H	4	0.19
(1,567)	1:145:A:ILE:HD13	1:171:A:ILE:H	4	0.19
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD11	5	0.19
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD12	5	0.19
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD13	5	0.19
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD21	5	0.19
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD22	5	0.19
(1,508)	1:136:A:VAL:H	1:155:A:LEU:HD23	5	0.19
(1,506)	1:136:A:VAL:H	1:148:A:SER:H	3	0.19
(1,454)	1:125:A:MET:H	1:128:A:ILE:HD11	1	0.19
(1,454)	1:125:A:MET:H	1:128:A:ILE:HD12	1	0.19
(1,454)	1:125:A:MET:H	1:128:A:ILE:HD13	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG11	7	0.19
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG12	7	0.19
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG13	7	0.19
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD11	5	0.19
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD12	5	0.19
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD13	5	0.19
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD21	5	0.19
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD22	5	0.19
(1,392)	1:107:A:TYR:H	1:109:A:LEU:HD23	5	0.19
(1,346)	1:84:A:ARG:H	1:86:A:GLY:H	3	0.19
(1,225)	1:55:A:GLN:H	1:58:A:ILE:H	4	0.19
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD11	7	0.19
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD12	7	0.19
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD13	7	0.19
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD21	7	0.19
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD22	7	0.19
(1,224)	1:55:A:GLN:H	1:57:A:LEU:HD23	7	0.19
(1,170)	1:49:A:LEU:HD11	1:109:A:LEU:H	1	0.19
(1,170)	1:49:A:LEU:HD12	1:109:A:LEU:H	1	0.19
(1,170)	1:49:A:LEU:HD13	1:109:A:LEU:H	1	0.19
(1,170)	1:49:A:LEU:HD21	1:109:A:LEU:H	1	0.19
(1,170)	1:49:A:LEU:HD22	1:109:A:LEU:H	1	0.19
(1,170)	1:49:A:LEU:HD23	1:109:A:LEU:H	1	0.19
(1,153)	1:47:A:CYS:H	1:52:A:GLU:H	4	0.19
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD11	1	0.19
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD12	1	0.19
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD13	1	0.19
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD11	5	0.19
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD12	5	0.19
(1,143)	1:45:A:VAL:H	1:67:A:ILE:HD13	5	0.19
(1,62)	1:32:A:PHE:H	1:66:A:ILE:HD11	7	0.19
(1,62)	1:32:A:PHE:H	1:66:A:ILE:HD12	7	0.19
(1,62)	1:32:A:PHE:H	1:66:A:ILE:HD13	7	0.19
(1,52)	1:32:A:PHE:H	1:135:A:LEU:H	7	0.19
(1,46)	1:31:A:LEU:H	1:65:A:LEU:H	6	0.19
(1,784)	1:184:A:CYS:HG	1:191:A:LEU:HD11	4	0.18
(1,784)	1:184:A:CYS:HG	1:191:A:LEU:HD12	4	0.18
(1,784)	1:184:A:CYS:HG	1:191:A:LEU:HD13	4	0.18
(1,765)	1:182:A:TRP:HE1	1:197:A:ALA:H	5	0.18
(1,743)	1:178:A:LEU:H	1:181:A:VAL:H	8	0.18
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD11	8	0.18
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD12	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD13	8	0.18
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD21	8	0.18
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD22	8	0.18
(1,676)	1:159:A:VAL:H	1:191:A:LEU:HD23	8	0.18
(1,638)	1:156:A:ILE:HD11	1:201:A:GLU:H	7	0.18
(1,638)	1:156:A:ILE:HD12	1:201:A:GLU:H	7	0.18
(1,638)	1:156:A:ILE:HD13	1:201:A:GLU:H	7	0.18
(1,632)	1:156:A:ILE:HD11	1:196:A:ARG:H	10	0.18
(1,632)	1:156:A:ILE:HD12	1:196:A:ARG:H	10	0.18
(1,632)	1:156:A:ILE:HD13	1:196:A:ARG:H	10	0.18
(1,618)	1:155:A:LEU:HD11	1:156:A:ILE:H	6	0.18
(1,618)	1:155:A:LEU:HD12	1:156:A:ILE:H	6	0.18
(1,618)	1:155:A:LEU:HD13	1:156:A:ILE:H	6	0.18
(1,506)	1:136:A:VAL:H	1:148:A:SER:H	10	0.18
(1,495)	1:135:A:LEU:HD11	1:153:A:LYS:H	2	0.18
(1,495)	1:135:A:LEU:HD12	1:153:A:LYS:H	2	0.18
(1,495)	1:135:A:LEU:HD13	1:153:A:LYS:H	2	0.18
(1,495)	1:135:A:LEU:HD21	1:153:A:LYS:H	2	0.18
(1,495)	1:135:A:LEU:HD22	1:153:A:LYS:H	2	0.18
(1,495)	1:135:A:LEU:HD23	1:153:A:LYS:H	2	0.18
(1,444)	1:116:A:VAL:H	1:118:A:GLY:H	2	0.18
(1,408)	1:108:A:VAL:H	1:112:A:GLY:H	6	0.18
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG21	9	0.18
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG22	9	0.18
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG23	9	0.18
(1,322)	1:81:A:VAL:HG11	1:116:A:VAL:H	6	0.18
(1,322)	1:81:A:VAL:HG12	1:116:A:VAL:H	6	0.18
(1,322)	1:81:A:VAL:HG13	1:116:A:VAL:H	6	0.18
(1,322)	1:81:A:VAL:HG21	1:116:A:VAL:H	6	0.18
(1,322)	1:81:A:VAL:HG22	1:116:A:VAL:H	6	0.18
(1,322)	1:81:A:VAL:HG23	1:116:A:VAL:H	6	0.18
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG11	6	0.18
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG12	6	0.18
(1,307)	1:80:A:LEU:H	1:81:A:VAL:HG13	6	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG11	1	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG12	1	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG13	1	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG21	1	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG22	1	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG23	1	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG11	1	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG12	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG13	1	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG21	1	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG22	1	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG23	1	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG11	1	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG12	1	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG13	1	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG21	1	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG22	1	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG23	1	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG11	1	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG12	1	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG13	1	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG21	1	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG22	1	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG23	1	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG11	1	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG12	1	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG13	1	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG21	1	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG22	1	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG23	1	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG11	1	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG12	1	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG13	1	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG21	1	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG22	1	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG23	1	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG11	7	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG12	7	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG13	7	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG21	7	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG22	7	0.18
(1,306)	1:80:A:LEU:HD11	1:81:A:VAL:HG23	7	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG11	7	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG12	7	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG13	7	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG21	7	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG22	7	0.18
(1,306)	1:80:A:LEU:HD12	1:81:A:VAL:HG23	7	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG11	7	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG12	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG13	7	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG21	7	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG22	7	0.18
(1,306)	1:80:A:LEU:HD13	1:81:A:VAL:HG23	7	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG11	7	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG12	7	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG13	7	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG21	7	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG22	7	0.18
(1,306)	1:80:A:LEU:HD21	1:81:A:VAL:HG23	7	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG11	7	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG12	7	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG13	7	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG21	7	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG22	7	0.18
(1,306)	1:80:A:LEU:HD22	1:81:A:VAL:HG23	7	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG11	7	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG12	7	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG13	7	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG21	7	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG22	7	0.18
(1,306)	1:80:A:LEU:HD23	1:81:A:VAL:HG23	7	0.18
(1,288)	1:66:A:ILE:H	1:68:A:GLN:H	5	0.18
(1,257)	1:60:A:TYR:H	1:62:A:PHE:H	5	0.18
(1,225)	1:55:A:GLN:H	1:58:A:ILE:H	6	0.18
(1,208)	1:52:A:GLU:H	1:55:A:GLN:H	4	0.18
(1,193)	1:49:A:LEU:HD11	1:80:A:LEU:H	3	0.18
(1,193)	1:49:A:LEU:HD12	1:80:A:LEU:H	3	0.18
(1,193)	1:49:A:LEU:HD13	1:80:A:LEU:H	3	0.18
(1,193)	1:49:A:LEU:HD21	1:80:A:LEU:H	3	0.18
(1,193)	1:49:A:LEU:HD22	1:80:A:LEU:H	3	0.18
(1,193)	1:49:A:LEU:HD23	1:80:A:LEU:H	3	0.18
(1,172)	1:49:A:LEU:HD11	1:116:A:VAL:H	10	0.18
(1,172)	1:49:A:LEU:HD12	1:116:A:VAL:H	10	0.18
(1,172)	1:49:A:LEU:HD13	1:116:A:VAL:H	10	0.18
(1,168)	1:49:A:LEU:HD11	1:107:A:TYR:H	1	0.18
(1,168)	1:49:A:LEU:HD12	1:107:A:TYR:H	1	0.18
(1,168)	1:49:A:LEU:HD13	1:107:A:TYR:H	1	0.18
(1,51)	1:32:A:PHE:H	1:134:A:ASP:H	10	0.18
(1,46)	1:31:A:LEU:H	1:65:A:LEU:H	3	0.18
(1,6)	1:25:A:ILE:H	1:27:A:GLU:H	5	0.18
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD11	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD12	5	0.17
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD13	5	0.17
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD21	5	0.17
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD22	5	0.17
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD23	5	0.17
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD11	5	0.17
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD12	5	0.17
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD13	5	0.17
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD21	5	0.17
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD22	5	0.17
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD23	5	0.17
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	1	0.17
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	1	0.17
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	8	0.17
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	8	0.17
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	10	0.17
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	10	0.17
(1,679)	1:162:A:SER:H	1:163:A:LEU:HD11	7	0.17
(1,679)	1:162:A:SER:H	1:163:A:LEU:HD12	7	0.17
(1,679)	1:162:A:SER:H	1:163:A:LEU:HD13	7	0.17
(1,679)	1:162:A:SER:H	1:163:A:LEU:HD21	7	0.17
(1,679)	1:162:A:SER:H	1:163:A:LEU:HD22	7	0.17
(1,679)	1:162:A:SER:H	1:163:A:LEU:HD23	7	0.17
(1,671)	1:159:A:VAL:HB	1:183:A:SER:H	10	0.17
(1,670)	1:159:A:VAL:HG11	1:181:A:VAL:H	6	0.17
(1,670)	1:159:A:VAL:HG12	1:181:A:VAL:H	6	0.17
(1,670)	1:159:A:VAL:HG13	1:181:A:VAL:H	6	0.17
(1,670)	1:159:A:VAL:HG21	1:181:A:VAL:H	6	0.17
(1,670)	1:159:A:VAL:HG22	1:181:A:VAL:H	6	0.17
(1,670)	1:159:A:VAL:HG23	1:181:A:VAL:H	6	0.17
(1,668)	1:159:A:VAL:HG11	1:175:A:PHE:H	10	0.17
(1,668)	1:159:A:VAL:HG12	1:175:A:PHE:H	10	0.17
(1,668)	1:159:A:VAL:HG13	1:175:A:PHE:H	10	0.17
(1,668)	1:159:A:VAL:HG21	1:175:A:PHE:H	10	0.17
(1,668)	1:159:A:VAL:HG22	1:175:A:PHE:H	10	0.17
(1,668)	1:159:A:VAL:HG23	1:175:A:PHE:H	10	0.17
(1,597)	1:149:A:LEU:H	1:153:A:LYS:H	2	0.17
(1,568)	1:145:A:ILE:HD11	1:172:A:ALA:H	6	0.17
(1,568)	1:145:A:ILE:HD12	1:172:A:ALA:H	6	0.17
(1,568)	1:145:A:ILE:HD13	1:172:A:ALA:H	6	0.17
(1,487)	1:134:A:ASP:H	1:136:A:VAL:H	6	0.17
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD11	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD12	1	0.17
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD13	1	0.17
(1,457)	1:126:A:GLN:H	1:129:A:ILE:H	8	0.17
(1,427)	1:110:A:MET:H	1:114:A:LEU:H	5	0.17
(1,412)	1:108:A:VAL:HG21	1:115:A:LYS:H	3	0.17
(1,412)	1:108:A:VAL:HG22	1:115:A:LYS:H	3	0.17
(1,412)	1:108:A:VAL:HG23	1:115:A:LYS:H	3	0.17
(1,369)	1:95:A:ILE:HD11	1:98:A:PHE:HD1	8	0.17
(1,369)	1:95:A:ILE:HD11	1:98:A:PHE:HD2	8	0.17
(1,369)	1:95:A:ILE:HD12	1:98:A:PHE:HD1	8	0.17
(1,369)	1:95:A:ILE:HD12	1:98:A:PHE:HD2	8	0.17
(1,369)	1:95:A:ILE:HD13	1:98:A:PHE:HD1	8	0.17
(1,369)	1:95:A:ILE:HD13	1:98:A:PHE:HD2	8	0.17
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG21	3	0.17
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG22	3	0.17
(1,362)	1:89:A:GLU:H	1:117:A:ILE:HG23	3	0.17
(1,353)	1:87:A:GLN:H	1:109:A:LEU:H	1	0.17
(1,346)	1:84:A:ARG:H	1:86:A:GLY:H	8	0.17
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD11	2	0.17
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD12	2	0.17
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD13	2	0.17
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD21	2	0.17
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD22	2	0.17
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD23	2	0.17
(1,326)	1:81:A:VAL:HG11	1:118:A:GLY:H	4	0.17
(1,326)	1:81:A:VAL:HG12	1:118:A:GLY:H	4	0.17
(1,326)	1:81:A:VAL:HG13	1:118:A:GLY:H	4	0.17
(1,326)	1:81:A:VAL:HG21	1:118:A:GLY:H	4	0.17
(1,326)	1:81:A:VAL:HG22	1:118:A:GLY:H	4	0.17
(1,326)	1:81:A:VAL:HG23	1:118:A:GLY:H	4	0.17
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG11	8	0.17
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG12	8	0.17
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG13	8	0.17
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG21	8	0.17
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG22	8	0.17
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG23	8	0.17
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG11	8	0.17
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG12	8	0.17
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG13	8	0.17
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG21	8	0.17
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG22	8	0.17
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG23	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	7	0.17
(1,169)	1:49:A:LEU:HD21	1:107:A:TYR:H	7	0.17
(1,169)	1:49:A:LEU:HD22	1:107:A:TYR:H	7	0.17
(1,169)	1:49:A:LEU:HD23	1:107:A:TYR:H	7	0.17
(1,86)	1:34:A:THR:H	1:139:A:HIS:H	5	0.17
(1,83)	1:34:A:THR:H	1:137:A:ILE:H	8	0.17
(1,30)	1:31:A:LEU:HD11	1:135:A:LEU:H	2	0.17
(1,30)	1:31:A:LEU:HD12	1:135:A:LEU:H	2	0.17
(1,30)	1:31:A:LEU:HD13	1:135:A:LEU:H	2	0.17
(1,30)	1:31:A:LEU:HD21	1:135:A:LEU:H	2	0.17
(1,30)	1:31:A:LEU:HD22	1:135:A:LEU:H	2	0.17
(1,30)	1:31:A:LEU:HD23	1:135:A:LEU:H	2	0.17
(1,27)	1:30:A:ALA:H	1:63:A:VAL:H	1	0.17
(1,890)	1:218:A:LEU:H	1:220:A:GLU:H	10	0.16
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD11	7	0.16
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD12	7	0.16
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD13	7	0.16
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD21	7	0.16
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD22	7	0.16
(1,875)	1:211:A:ASN:HD21	1:218:A:LEU:HD23	7	0.16
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD11	7	0.16
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD12	7	0.16
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD13	7	0.16
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD21	7	0.16
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD22	7	0.16
(1,875)	1:211:A:ASN:HD22	1:218:A:LEU:HD23	7	0.16
(1,821)	1:191:A:LEU:HD21	1:194:A:GLY:H	5	0.16
(1,821)	1:191:A:LEU:HD22	1:194:A:GLY:H	5	0.16
(1,821)	1:191:A:LEU:HD23	1:194:A:GLY:H	5	0.16
(1,782)	1:184:A:CYS:HG	1:187:A:THR:H	4	0.16
(1,774)	1:182:A:TRP:H	1:203:A:LEU:HD11	9	0.16
(1,774)	1:182:A:TRP:H	1:203:A:LEU:HD12	9	0.16
(1,774)	1:182:A:TRP:H	1:203:A:LEU:HD13	9	0.16
(1,765)	1:182:A:TRP:HE1	1:197:A:ALA:H	4	0.16
(1,761)	1:181:A:VAL:H	1:183:A:SER:H	1	0.16
(1,747)	1:179:A:GLY:H	1:203:A:LEU:HD11	6	0.16
(1,747)	1:179:A:GLY:H	1:203:A:LEU:HD12	6	0.16
(1,747)	1:179:A:GLY:H	1:203:A:LEU:HD13	6	0.16
(1,677)	1:161:A:ASP:H	1:163:A:LEU:H	9	0.16
(1,652)	1:157:A:VAL:H	1:184:A:CYS:HG	4	0.16
(1,645)	1:157:A:VAL:H	1:159:A:VAL:HB	10	0.16
(1,638)	1:156:A:ILE:HD11	1:201:A:GLU:H	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:156:A:ILE:HD12	1:201:A:GLU:H	9	0.16
(1,638)	1:156:A:ILE:HD13	1:201:A:GLU:H	9	0.16
(1,597)	1:149:A:LEU:H	1:153:A:LYS:H	7	0.16
(1,551)	1:144:A:SER:H	1:145:A:ILE:HD11	5	0.16
(1,551)	1:144:A:SER:H	1:145:A:ILE:HD12	5	0.16
(1,551)	1:144:A:SER:H	1:145:A:ILE:HD13	5	0.16
(1,534)	1:139:A:HIS:H	1:157:A:VAL:HG21	8	0.16
(1,534)	1:139:A:HIS:H	1:157:A:VAL:HG22	8	0.16
(1,534)	1:139:A:HIS:H	1:157:A:VAL:HG23	8	0.16
(1,529)	1:139:A:HIS:H	1:140:A:ALA:H	8	0.16
(1,495)	1:135:A:LEU:HD11	1:153:A:LYS:H	9	0.16
(1,495)	1:135:A:LEU:HD12	1:153:A:LYS:H	9	0.16
(1,495)	1:135:A:LEU:HD13	1:153:A:LYS:H	9	0.16
(1,495)	1:135:A:LEU:HD21	1:153:A:LYS:H	9	0.16
(1,495)	1:135:A:LEU:HD22	1:153:A:LYS:H	9	0.16
(1,495)	1:135:A:LEU:HD23	1:153:A:LYS:H	9	0.16
(1,480)	1:130:A:ARG:H	1:151:A:LEU:HD11	4	0.16
(1,480)	1:130:A:ARG:H	1:151:A:LEU:HD12	4	0.16
(1,480)	1:130:A:ARG:H	1:151:A:LEU:HD13	4	0.16
(1,480)	1:130:A:ARG:H	1:151:A:LEU:HD21	4	0.16
(1,480)	1:130:A:ARG:H	1:151:A:LEU:HD22	4	0.16
(1,480)	1:130:A:ARG:H	1:151:A:LEU:HD23	4	0.16
(1,473)	1:129:A:ILE:H	1:133:A:SER:H	4	0.16
(1,457)	1:126:A:GLN:H	1:129:A:ILE:H	5	0.16
(1,412)	1:108:A:VAL:HG21	1:115:A:LYS:H	1	0.16
(1,412)	1:108:A:VAL:HG22	1:115:A:LYS:H	1	0.16
(1,412)	1:108:A:VAL:HG23	1:115:A:LYS:H	1	0.16
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG11	3	0.16
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG12	3	0.16
(1,399)	1:108:A:VAL:H	1:108:A:VAL:HG13	3	0.16
(1,337)	1:81:A:VAL:HG11	1:89:A:GLU:H	4	0.16
(1,337)	1:81:A:VAL:HG12	1:89:A:GLU:H	4	0.16
(1,337)	1:81:A:VAL:HG13	1:89:A:GLU:H	4	0.16
(1,337)	1:81:A:VAL:HG21	1:89:A:GLU:H	4	0.16
(1,337)	1:81:A:VAL:HG22	1:89:A:GLU:H	4	0.16
(1,337)	1:81:A:VAL:HG23	1:89:A:GLU:H	4	0.16
(1,263)	1:63:A:VAL:H	1:115:A:LYS:H	10	0.16
(1,262)	1:63:A:VAL:HG11	1:115:A:LYS:H	10	0.16
(1,262)	1:63:A:VAL:HG12	1:115:A:LYS:H	10	0.16
(1,262)	1:63:A:VAL:HG13	1:115:A:LYS:H	10	0.16
(1,262)	1:63:A:VAL:HG21	1:115:A:LYS:H	10	0.16
(1,262)	1:63:A:VAL:HG22	1:115:A:LYS:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:63:A:VAL:HG23	1:115:A:LYS:H	10	0.16
(1,241)	1:57:A:LEU:HD11	1:59:A:GLN:H	3	0.16
(1,241)	1:57:A:LEU:HD12	1:59:A:GLN:H	3	0.16
(1,241)	1:57:A:LEU:HD13	1:59:A:GLN:H	3	0.16
(1,241)	1:57:A:LEU:HD21	1:59:A:GLN:H	3	0.16
(1,241)	1:57:A:LEU:HD22	1:59:A:GLN:H	3	0.16
(1,241)	1:57:A:LEU:HD23	1:59:A:GLN:H	3	0.16
(1,225)	1:55:A:GLN:H	1:58:A:ILE:H	3	0.16
(1,204)	1:51:A:ASP:H	1:54:A:CYS:H	10	0.16
(1,193)	1:49:A:LEU:HD11	1:80:A:LEU:H	10	0.16
(1,193)	1:49:A:LEU:HD12	1:80:A:LEU:H	10	0.16
(1,193)	1:49:A:LEU:HD13	1:80:A:LEU:H	10	0.16
(1,193)	1:49:A:LEU:HD21	1:80:A:LEU:H	10	0.16
(1,193)	1:49:A:LEU:HD22	1:80:A:LEU:H	10	0.16
(1,193)	1:49:A:LEU:HD23	1:80:A:LEU:H	10	0.16
(1,180)	1:49:A:LEU:HD11	1:118:A:GLY:H	3	0.16
(1,180)	1:49:A:LEU:HD12	1:118:A:GLY:H	3	0.16
(1,180)	1:49:A:LEU:HD13	1:118:A:GLY:H	3	0.16
(1,180)	1:49:A:LEU:HD21	1:118:A:GLY:H	3	0.16
(1,180)	1:49:A:LEU:HD22	1:118:A:GLY:H	3	0.16
(1,180)	1:49:A:LEU:HD23	1:118:A:GLY:H	3	0.16
(1,104)	1:39:A:VAL:HG11	1:46:A:SER:H	3	0.16
(1,104)	1:39:A:VAL:HG12	1:46:A:SER:H	3	0.16
(1,104)	1:39:A:VAL:HG13	1:46:A:SER:H	3	0.16
(1,104)	1:39:A:VAL:HG21	1:46:A:SER:H	3	0.16
(1,104)	1:39:A:VAL:HG22	1:46:A:SER:H	3	0.16
(1,104)	1:39:A:VAL:HG23	1:46:A:SER:H	3	0.16
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD11	7	0.16
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD12	7	0.16
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD13	7	0.16
(1,46)	1:31:A:LEU:H	1:65:A:LEU:H	1	0.16
(1,29)	1:31:A:LEU:HD11	1:134:A:ASP:H	5	0.16
(1,29)	1:31:A:LEU:HD12	1:134:A:ASP:H	5	0.16
(1,29)	1:31:A:LEU:HD13	1:134:A:ASP:H	5	0.16
(1,29)	1:31:A:LEU:HD21	1:134:A:ASP:H	5	0.16
(1,29)	1:31:A:LEU:HD22	1:134:A:ASP:H	5	0.16
(1,29)	1:31:A:LEU:HD23	1:134:A:ASP:H	5	0.16
(1,23)	1:30:A:ALA:H	1:135:A:LEU:H	3	0.16
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE1	7	0.16
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE2	7	0.16
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE1	7	0.16
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE2	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE1	7	0.16
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE2	7	0.16
(1,3)	1:25:A:ILE:H	1:26:A:ILE:H	10	0.16
(1,1)	1:25:A:ILE:HD11	1:26:A:ILE:H	7	0.16
(1,1)	1:25:A:ILE:HD12	1:26:A:ILE:H	7	0.16
(1,1)	1:25:A:ILE:HD13	1:26:A:ILE:H	7	0.16
(1,901)	1:223:A:TYR:H	1:224:A:SER:H	7	0.15
(1,890)	1:218:A:LEU:H	1:220:A:GLU:H	7	0.15
(1,890)	1:218:A:LEU:H	1:220:A:GLU:H	9	0.15
(1,859)	1:200:A:THR:H	1:201:A:GLU:H	10	0.15
(1,838)	1:195:A:LEU:HD11	1:198:A:SER:H	2	0.15
(1,838)	1:195:A:LEU:HD12	1:198:A:SER:H	2	0.15
(1,838)	1:195:A:LEU:HD13	1:198:A:SER:H	2	0.15
(1,838)	1:195:A:LEU:HD21	1:198:A:SER:H	2	0.15
(1,838)	1:195:A:LEU:HD22	1:198:A:SER:H	2	0.15
(1,838)	1:195:A:LEU:HD23	1:198:A:SER:H	2	0.15
(1,794)	1:187:A:THR:H	1:189:A:THR:H	8	0.15
(1,777)	1:183:A:SER:H	1:184:A:CYS:HG	9	0.15
(1,772)	1:182:A:TRP:HE1	1:203:A:LEU:H	3	0.15
(1,761)	1:181:A:VAL:H	1:183:A:SER:H	2	0.15
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG21	6	0.15
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG22	6	0.15
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG23	6	0.15
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG21	9	0.15
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG22	9	0.15
(1,713)	1:175:A:PHE:H	1:181:A:VAL:HG23	9	0.15
(1,677)	1:161:A:ASP:H	1:163:A:LEU:H	10	0.15
(1,664)	1:159:A:VAL:HG21	1:172:A:ALA:H	7	0.15
(1,664)	1:159:A:VAL:HG22	1:172:A:ALA:H	7	0.15
(1,664)	1:159:A:VAL:HG23	1:172:A:ALA:H	7	0.15
(1,538)	1:140:A:ALA:H	1:145:A:ILE:HD11	3	0.15
(1,538)	1:140:A:ALA:H	1:145:A:ILE:HD12	3	0.15
(1,538)	1:140:A:ALA:H	1:145:A:ILE:HD13	3	0.15
(1,511)	1:136:A:VAL:H	1:156:A:ILE:HD11	8	0.15
(1,511)	1:136:A:VAL:H	1:156:A:ILE:HD12	8	0.15
(1,511)	1:136:A:VAL:H	1:156:A:ILE:HD13	8	0.15
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD11	4	0.15
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD12	4	0.15
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD13	4	0.15
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD11	8	0.15
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD12	8	0.15
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD13	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:81:A:VAL:HG11	1:98:A:PHE:HD1	3	0.15
(1,338)	1:81:A:VAL:HG11	1:98:A:PHE:HD2	3	0.15
(1,338)	1:81:A:VAL:HG12	1:98:A:PHE:HD1	3	0.15
(1,338)	1:81:A:VAL:HG12	1:98:A:PHE:HD2	3	0.15
(1,338)	1:81:A:VAL:HG13	1:98:A:PHE:HD1	3	0.15
(1,338)	1:81:A:VAL:HG13	1:98:A:PHE:HD2	3	0.15
(1,338)	1:81:A:VAL:HG21	1:98:A:PHE:HD1	3	0.15
(1,338)	1:81:A:VAL:HG21	1:98:A:PHE:HD2	3	0.15
(1,338)	1:81:A:VAL:HG22	1:98:A:PHE:HD1	3	0.15
(1,338)	1:81:A:VAL:HG22	1:98:A:PHE:HD2	3	0.15
(1,338)	1:81:A:VAL:HG23	1:98:A:PHE:HD1	3	0.15
(1,338)	1:81:A:VAL:HG23	1:98:A:PHE:HD2	3	0.15
(1,325)	1:81:A:VAL:HG11	1:117:A:ILE:H	2	0.15
(1,325)	1:81:A:VAL:HG12	1:117:A:ILE:H	2	0.15
(1,325)	1:81:A:VAL:HG13	1:117:A:ILE:H	2	0.15
(1,325)	1:81:A:VAL:HG21	1:117:A:ILE:H	2	0.15
(1,325)	1:81:A:VAL:HG22	1:117:A:ILE:H	2	0.15
(1,325)	1:81:A:VAL:HG23	1:117:A:ILE:H	2	0.15
(1,294)	1:67:A:ILE:HD11	1:69:A:PHE:HD1	5	0.15
(1,294)	1:67:A:ILE:HD11	1:69:A:PHE:HD2	5	0.15
(1,294)	1:67:A:ILE:HD12	1:69:A:PHE:HD1	5	0.15
(1,294)	1:67:A:ILE:HD12	1:69:A:PHE:HD2	5	0.15
(1,294)	1:67:A:ILE:HD13	1:69:A:PHE:HD1	5	0.15
(1,294)	1:67:A:ILE:HD13	1:69:A:PHE:HD2	5	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG11	7	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG12	7	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG13	7	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG21	7	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG22	7	0.15
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG23	7	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG11	7	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG12	7	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG13	7	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG21	7	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG22	7	0.15
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG23	7	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG11	7	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG12	7	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG13	7	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG21	7	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG22	7	0.15
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG23	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG11	7	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG12	7	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG13	7	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG21	7	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG22	7	0.15
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG23	7	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG11	7	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG12	7	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG13	7	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG21	7	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG22	7	0.15
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG23	7	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG11	7	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG12	7	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG13	7	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG21	7	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG22	7	0.15
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG23	7	0.15
(1,271)	1:64:A:ARG:H	1:115:A:LYS:H	5	0.15
(1,257)	1:60:A:TYR:H	1:62:A:PHE:H	10	0.15
(1,225)	1:55:A:GLN:H	1:58:A:ILE:H	8	0.15
(1,204)	1:51:A:ASP:H	1:54:A:CYS:H	2	0.15
(1,203)	1:51:A:ASP:H	1:53:A:PHE:H	4	0.15
(1,190)	1:49:A:LEU:HD11	1:77:A:PHE:HD1	3	0.15
(1,190)	1:49:A:LEU:HD11	1:77:A:PHE:HD2	3	0.15
(1,190)	1:49:A:LEU:HD12	1:77:A:PHE:HD1	3	0.15
(1,190)	1:49:A:LEU:HD12	1:77:A:PHE:HD2	3	0.15
(1,190)	1:49:A:LEU:HD13	1:77:A:PHE:HD1	3	0.15
(1,190)	1:49:A:LEU:HD13	1:77:A:PHE:HD2	3	0.15
(1,189)	1:49:A:LEU:H	1:67:A:ILE:HD11	8	0.15
(1,189)	1:49:A:LEU:H	1:67:A:ILE:HD12	8	0.15
(1,189)	1:49:A:LEU:H	1:67:A:ILE:HD13	8	0.15
(1,168)	1:49:A:LEU:HD11	1:107:A:TYR:H	6	0.15
(1,168)	1:49:A:LEU:HD12	1:107:A:TYR:H	6	0.15
(1,168)	1:49:A:LEU:HD13	1:107:A:TYR:H	6	0.15
(1,100)	1:39:A:VAL:HG11	1:43:A:LYS:H	2	0.15
(1,100)	1:39:A:VAL:HG12	1:43:A:LYS:H	2	0.15
(1,100)	1:39:A:VAL:HG13	1:43:A:LYS:H	2	0.15
(1,100)	1:39:A:VAL:HG21	1:43:A:LYS:H	2	0.15
(1,100)	1:39:A:VAL:HG22	1:43:A:LYS:H	2	0.15
(1,100)	1:39:A:VAL:HG23	1:43:A:LYS:H	2	0.15
(1,97)	1:35:A:CYS:H	1:68:A:GLN:H	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:35:A:CYS:H	1:67:A:ILE:HG21	5	0.15
(1,95)	1:35:A:CYS:H	1:67:A:ILE:HG22	5	0.15
(1,95)	1:35:A:CYS:H	1:67:A:ILE:HG23	5	0.15
(1,71)	1:33:A:VAL:HG21	1:34:A:THR:H	6	0.15
(1,71)	1:33:A:VAL:HG22	1:34:A:THR:H	6	0.15
(1,71)	1:33:A:VAL:HG23	1:34:A:THR:H	6	0.15
(1,63)	1:33:A:VAL:HG11	1:137:A:ILE:H	3	0.15
(1,63)	1:33:A:VAL:HG12	1:137:A:ILE:H	3	0.15
(1,63)	1:33:A:VAL:HG13	1:137:A:ILE:H	3	0.15
(1,63)	1:33:A:VAL:HG21	1:137:A:ILE:H	3	0.15
(1,63)	1:33:A:VAL:HG22	1:137:A:ILE:H	3	0.15
(1,63)	1:33:A:VAL:HG23	1:137:A:ILE:H	3	0.15
(1,63)	1:33:A:VAL:HG11	1:137:A:ILE:H	9	0.15
(1,63)	1:33:A:VAL:HG12	1:137:A:ILE:H	9	0.15
(1,63)	1:33:A:VAL:HG13	1:137:A:ILE:H	9	0.15
(1,63)	1:33:A:VAL:HG21	1:137:A:ILE:H	9	0.15
(1,63)	1:33:A:VAL:HG22	1:137:A:ILE:H	9	0.15
(1,63)	1:33:A:VAL:HG23	1:137:A:ILE:H	9	0.15
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD11	5	0.15
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD12	5	0.15
(1,49)	1:31:A:LEU:H	1:66:A:ILE:HD13	5	0.15
(1,46)	1:31:A:LEU:H	1:65:A:LEU:H	4	0.15
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD11	3	0.15
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD12	3	0.15
(1,33)	1:31:A:LEU:H	1:137:A:ILE:HD13	3	0.15
(1,27)	1:30:A:ALA:H	1:63:A:VAL:H	10	0.15
(1,23)	1:30:A:ALA:H	1:135:A:LEU:H	9	0.15
(1,19)	1:30:A:ALA:H	1:133:A:SER:H	6	0.15
(1,890)	1:218:A:LEU:H	1:220:A:GLU:H	3	0.14
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	5	0.14
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	5	0.14
(1,794)	1:187:A:THR:H	1:189:A:THR:H	7	0.14
(1,765)	1:182:A:TRP:HE1	1:197:A:ALA:H	9	0.14
(1,741)	1:178:A:LEU:HD11	1:180:A:TYR:H	3	0.14
(1,741)	1:178:A:LEU:HD12	1:180:A:TYR:H	3	0.14
(1,741)	1:178:A:LEU:HD13	1:180:A:TYR:H	3	0.14
(1,741)	1:178:A:LEU:HD21	1:180:A:TYR:H	3	0.14
(1,741)	1:178:A:LEU:HD22	1:180:A:TYR:H	3	0.14
(1,741)	1:178:A:LEU:HD23	1:180:A:TYR:H	3	0.14
(1,731)	1:176:A:VAL:HG11	1:183:A:SER:H	1	0.14
(1,731)	1:176:A:VAL:HG12	1:183:A:SER:H	1	0.14
(1,731)	1:176:A:VAL:HG13	1:183:A:SER:H	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,731)	1:176:A:VAL:HG21	1:183:A:SER:H	1	0.14
(1,731)	1:176:A:VAL:HG22	1:183:A:SER:H	1	0.14
(1,731)	1:176:A:VAL:HG23	1:183:A:SER:H	1	0.14
(1,677)	1:161:A:ASP:H	1:163:A:LEU:H	8	0.14
(1,670)	1:159:A:VAL:HG11	1:181:A:VAL:H	1	0.14
(1,670)	1:159:A:VAL:HG12	1:181:A:VAL:H	1	0.14
(1,670)	1:159:A:VAL:HG13	1:181:A:VAL:H	1	0.14
(1,670)	1:159:A:VAL:HG21	1:181:A:VAL:H	1	0.14
(1,670)	1:159:A:VAL:HG22	1:181:A:VAL:H	1	0.14
(1,670)	1:159:A:VAL:HG23	1:181:A:VAL:H	1	0.14
(1,650)	1:157:A:VAL:H	1:183:A:SER:H	5	0.14
(1,627)	1:156:A:ILE:HD11	1:191:A:LEU:HD11	7	0.14
(1,627)	1:156:A:ILE:HD11	1:191:A:LEU:HD12	7	0.14
(1,627)	1:156:A:ILE:HD11	1:191:A:LEU:HD13	7	0.14
(1,627)	1:156:A:ILE:HD11	1:191:A:LEU:HD21	7	0.14
(1,627)	1:156:A:ILE:HD11	1:191:A:LEU:HD22	7	0.14
(1,627)	1:156:A:ILE:HD11	1:191:A:LEU:HD23	7	0.14
(1,627)	1:156:A:ILE:HD12	1:191:A:LEU:HD11	7	0.14
(1,627)	1:156:A:ILE:HD12	1:191:A:LEU:HD12	7	0.14
(1,627)	1:156:A:ILE:HD12	1:191:A:LEU:HD13	7	0.14
(1,627)	1:156:A:ILE:HD12	1:191:A:LEU:HD21	7	0.14
(1,627)	1:156:A:ILE:HD12	1:191:A:LEU:HD22	7	0.14
(1,627)	1:156:A:ILE:HD12	1:191:A:LEU:HD23	7	0.14
(1,627)	1:156:A:ILE:HD13	1:191:A:LEU:HD11	7	0.14
(1,627)	1:156:A:ILE:HD13	1:191:A:LEU:HD12	7	0.14
(1,627)	1:156:A:ILE:HD13	1:191:A:LEU:HD13	7	0.14
(1,627)	1:156:A:ILE:HD13	1:191:A:LEU:HD21	7	0.14
(1,627)	1:156:A:ILE:HD13	1:191:A:LEU:HD22	7	0.14
(1,627)	1:156:A:ILE:HD13	1:191:A:LEU:HD23	7	0.14
(1,586)	1:148:A:SER:H	1:152:A:ASN:H	6	0.14
(1,526)	1:138:A:SER:H	1:157:A:VAL:H	9	0.14
(1,463)	1:127:A:SER:H	1:130:A:ARG:H	2	0.14
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD11	9	0.14
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD12	9	0.14
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD13	9	0.14
(1,447)	1:117:A:ILE:HD11	1:118:A:GLY:H	3	0.14
(1,447)	1:117:A:ILE:HD12	1:118:A:GLY:H	3	0.14
(1,447)	1:117:A:ILE:HD13	1:118:A:GLY:H	3	0.14
(1,419)	1:109:A:LEU:H	1:113:A:LYS:H	4	0.14
(1,405)	1:108:A:VAL:H	1:110:A:MET:H	3	0.14
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD11	9	0.14
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD12	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:107:A:TYR:H	1:117:A:ILE:HD13	9	0.14
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD11	8	0.14
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD12	8	0.14
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD13	8	0.14
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD21	8	0.14
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD22	8	0.14
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD23	8	0.14
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG11	2	0.14
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG12	2	0.14
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG13	2	0.14
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG21	2	0.14
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG22	2	0.14
(1,298)	1:77:A:PHE:HD1	1:116:A:VAL:HG23	2	0.14
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG11	2	0.14
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG12	2	0.14
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG13	2	0.14
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG21	2	0.14
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG22	2	0.14
(1,298)	1:77:A:PHE:HD2	1:116:A:VAL:HG23	2	0.14
(1,294)	1:67:A:ILE:HD11	1:69:A:PHE:HD1	4	0.14
(1,294)	1:67:A:ILE:HD11	1:69:A:PHE:HD2	4	0.14
(1,294)	1:67:A:ILE:HD12	1:69:A:PHE:HD1	4	0.14
(1,294)	1:67:A:ILE:HD12	1:69:A:PHE:HD2	4	0.14
(1,294)	1:67:A:ILE:HD13	1:69:A:PHE:HD1	4	0.14
(1,294)	1:67:A:ILE:HD13	1:69:A:PHE:HD2	4	0.14
(1,291)	1:67:A:ILE:H	1:118:A:GLY:H	10	0.14
(1,247)	1:57:A:LEU:HD11	1:62:A:PHE:HE1	10	0.14
(1,247)	1:57:A:LEU:HD11	1:62:A:PHE:HE2	10	0.14
(1,247)	1:57:A:LEU:HD12	1:62:A:PHE:HE1	10	0.14
(1,247)	1:57:A:LEU:HD12	1:62:A:PHE:HE2	10	0.14
(1,247)	1:57:A:LEU:HD13	1:62:A:PHE:HE1	10	0.14
(1,247)	1:57:A:LEU:HD13	1:62:A:PHE:HE2	10	0.14
(1,247)	1:57:A:LEU:HD21	1:62:A:PHE:HE1	10	0.14
(1,247)	1:57:A:LEU:HD21	1:62:A:PHE:HE2	10	0.14
(1,247)	1:57:A:LEU:HD22	1:62:A:PHE:HE1	10	0.14
(1,247)	1:57:A:LEU:HD22	1:62:A:PHE:HE2	10	0.14
(1,247)	1:57:A:LEU:HD23	1:62:A:PHE:HE1	10	0.14
(1,247)	1:57:A:LEU:HD23	1:62:A:PHE:HE2	10	0.14
(1,241)	1:57:A:LEU:HD11	1:59:A:GLN:H	1	0.14
(1,241)	1:57:A:LEU:HD12	1:59:A:GLN:H	1	0.14
(1,241)	1:57:A:LEU:HD13	1:59:A:GLN:H	1	0.14
(1,241)	1:57:A:LEU:HD21	1:59:A:GLN:H	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:57:A:LEU:HD22	1:59:A:GLN:H	1	0.14
(1,241)	1:57:A:LEU:HD23	1:59:A:GLN:H	1	0.14
(1,225)	1:55:A:GLN:H	1:58:A:ILE:H	10	0.14
(1,203)	1:51:A:ASP:H	1:53:A:PHE:H	10	0.14
(1,184)	1:49:A:LEU:H	1:51:A:ASP:H	1	0.14
(1,184)	1:49:A:LEU:H	1:51:A:ASP:H	5	0.14
(1,168)	1:49:A:LEU:HD11	1:107:A:TYR:H	3	0.14
(1,168)	1:49:A:LEU:HD12	1:107:A:TYR:H	3	0.14
(1,168)	1:49:A:LEU:HD13	1:107:A:TYR:H	3	0.14
(1,168)	1:49:A:LEU:HD11	1:107:A:TYR:H	9	0.14
(1,168)	1:49:A:LEU:HD12	1:107:A:TYR:H	9	0.14
(1,168)	1:49:A:LEU:HD13	1:107:A:TYR:H	9	0.14
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	2	0.14
(1,163)	1:48:A:VAL:H	1:52:A:GLU:H	3	0.14
(1,153)	1:47:A:CYS:H	1:52:A:GLU:H	2	0.14
(1,153)	1:47:A:CYS:H	1:52:A:GLU:H	9	0.14
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG11	3	0.14
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG12	3	0.14
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG13	3	0.14
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG21	3	0.14
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG22	3	0.14
(1,125)	1:44:A:LEU:HD11	1:45:A:VAL:HG23	3	0.14
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG11	3	0.14
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG12	3	0.14
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG13	3	0.14
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG21	3	0.14
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG22	3	0.14
(1,125)	1:44:A:LEU:HD12	1:45:A:VAL:HG23	3	0.14
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG11	3	0.14
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG12	3	0.14
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG13	3	0.14
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG21	3	0.14
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG22	3	0.14
(1,125)	1:44:A:LEU:HD13	1:45:A:VAL:HG23	3	0.14
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG11	3	0.14
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG12	3	0.14
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG13	3	0.14
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG21	3	0.14
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG22	3	0.14
(1,125)	1:44:A:LEU:HD21	1:45:A:VAL:HG23	3	0.14
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG11	3	0.14
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG12	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG13	3	0.14
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG21	3	0.14
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG22	3	0.14
(1,125)	1:44:A:LEU:HD22	1:45:A:VAL:HG23	3	0.14
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG11	3	0.14
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG12	3	0.14
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG13	3	0.14
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG21	3	0.14
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG22	3	0.14
(1,125)	1:44:A:LEU:HD23	1:45:A:VAL:HG23	3	0.14
(1,48)	1:31:A:LEU:H	1:66:A:ILE:H	3	0.14
(1,6)	1:25:A:ILE:H	1:27:A:GLU:H	4	0.14
(1,4)	1:25:A:ILE:HD11	1:27:A:GLU:H	1	0.14
(1,4)	1:25:A:ILE:HD12	1:27:A:GLU:H	1	0.14
(1,4)	1:25:A:ILE:HD13	1:27:A:GLU:H	1	0.14
(1,890)	1:218:A:LEU:H	1:220:A:GLU:H	8	0.13
(1,863)	1:203:A:LEU:H	1:203:A:LEU:HD21	3	0.13
(1,863)	1:203:A:LEU:H	1:203:A:LEU:HD22	3	0.13
(1,863)	1:203:A:LEU:H	1:203:A:LEU:HD23	3	0.13
(1,802)	1:188:A:GLU:H	1:192:A:ILE:HD11	8	0.13
(1,802)	1:188:A:GLU:H	1:192:A:ILE:HD12	8	0.13
(1,802)	1:188:A:GLU:H	1:192:A:ILE:HD13	8	0.13
(1,778)	1:184:A:CYS:H	1:184:A:CYS:HG	8	0.13
(1,774)	1:182:A:TRP:H	1:203:A:LEU:HD11	5	0.13
(1,774)	1:182:A:TRP:H	1:203:A:LEU:HD12	5	0.13
(1,774)	1:182:A:TRP:H	1:203:A:LEU:HD13	5	0.13
(1,765)	1:182:A:TRP:HE1	1:197:A:ALA:H	2	0.13
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG21	8	0.13
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG22	8	0.13
(1,751)	1:180:A:TYR:H	1:181:A:VAL:HG23	8	0.13
(1,743)	1:178:A:LEU:H	1:181:A:VAL:H	6	0.13
(1,741)	1:178:A:LEU:HD11	1:180:A:TYR:H	9	0.13
(1,741)	1:178:A:LEU:HD12	1:180:A:TYR:H	9	0.13
(1,741)	1:178:A:LEU:HD13	1:180:A:TYR:H	9	0.13
(1,741)	1:178:A:LEU:HD21	1:180:A:TYR:H	9	0.13
(1,741)	1:178:A:LEU:HD22	1:180:A:TYR:H	9	0.13
(1,741)	1:178:A:LEU:HD23	1:180:A:TYR:H	9	0.13
(1,635)	1:156:A:ILE:HG21	1:198:A:SER:H	8	0.13
(1,635)	1:156:A:ILE:HG22	1:198:A:SER:H	8	0.13
(1,635)	1:156:A:ILE:HG23	1:198:A:SER:H	8	0.13
(1,582)	1:147:A:ASP:H	1:155:A:LEU:HD11	9	0.13
(1,582)	1:147:A:ASP:H	1:155:A:LEU:HD12	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:147:A:ASP:H	1:155:A:LEU:HD13	9	0.13
(1,582)	1:147:A:ASP:H	1:155:A:LEU:HD21	9	0.13
(1,582)	1:147:A:ASP:H	1:155:A:LEU:HD22	9	0.13
(1,582)	1:147:A:ASP:H	1:155:A:LEU:HD23	9	0.13
(1,567)	1:145:A:ILE:HD11	1:171:A:ILE:H	10	0.13
(1,567)	1:145:A:ILE:HD12	1:171:A:ILE:H	10	0.13
(1,567)	1:145:A:ILE:HD13	1:171:A:ILE:H	10	0.13
(1,537)	1:140:A:ALA:H	1:141:A:GLY:H	2	0.13
(1,528)	1:138:A:SER:HG	1:158:A:CYS:H	3	0.13
(1,526)	1:138:A:SER:H	1:157:A:VAL:H	8	0.13
(1,505)	1:136:A:VAL:H	1:138:A:SER:H	2	0.13
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD11	5	0.13
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD12	5	0.13
(1,462)	1:127:A:SER:H	1:129:A:ILE:HD13	5	0.13
(1,427)	1:110:A:MET:H	1:114:A:LEU:H	9	0.13
(1,382)	1:105:A:ARG:H	1:107:A:TYR:H	10	0.13
(1,338)	1:81:A:VAL:HG11	1:98:A:PHE:HD1	5	0.13
(1,338)	1:81:A:VAL:HG11	1:98:A:PHE:HD2	5	0.13
(1,338)	1:81:A:VAL:HG12	1:98:A:PHE:HD1	5	0.13
(1,338)	1:81:A:VAL:HG12	1:98:A:PHE:HD2	5	0.13
(1,338)	1:81:A:VAL:HG13	1:98:A:PHE:HD1	5	0.13
(1,338)	1:81:A:VAL:HG13	1:98:A:PHE:HD2	5	0.13
(1,338)	1:81:A:VAL:HG21	1:98:A:PHE:HD1	5	0.13
(1,338)	1:81:A:VAL:HG21	1:98:A:PHE:HD2	5	0.13
(1,338)	1:81:A:VAL:HG22	1:98:A:PHE:HD1	5	0.13
(1,338)	1:81:A:VAL:HG22	1:98:A:PHE:HD2	5	0.13
(1,338)	1:81:A:VAL:HG23	1:98:A:PHE:HD1	5	0.13
(1,338)	1:81:A:VAL:HG23	1:98:A:PHE:HD2	5	0.13
(1,337)	1:81:A:VAL:HG11	1:89:A:GLU:H	7	0.13
(1,337)	1:81:A:VAL:HG12	1:89:A:GLU:H	7	0.13
(1,337)	1:81:A:VAL:HG13	1:89:A:GLU:H	7	0.13
(1,337)	1:81:A:VAL:HG21	1:89:A:GLU:H	7	0.13
(1,337)	1:81:A:VAL:HG22	1:89:A:GLU:H	7	0.13
(1,337)	1:81:A:VAL:HG23	1:89:A:GLU:H	7	0.13
(1,325)	1:81:A:VAL:HG11	1:117:A:ILE:H	1	0.13
(1,325)	1:81:A:VAL:HG12	1:117:A:ILE:H	1	0.13
(1,325)	1:81:A:VAL:HG13	1:117:A:ILE:H	1	0.13
(1,325)	1:81:A:VAL:HG21	1:117:A:ILE:H	1	0.13
(1,325)	1:81:A:VAL:HG22	1:117:A:ILE:H	1	0.13
(1,325)	1:81:A:VAL:HG23	1:117:A:ILE:H	1	0.13
(1,324)	1:81:A:VAL:H	1:116:A:VAL:HG11	6	0.13
(1,324)	1:81:A:VAL:H	1:116:A:VAL:HG12	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:81:A:VAL:H	1:116:A:VAL:HG13	6	0.13
(1,324)	1:81:A:VAL:H	1:116:A:VAL:HG21	6	0.13
(1,324)	1:81:A:VAL:H	1:116:A:VAL:HG22	6	0.13
(1,324)	1:81:A:VAL:H	1:116:A:VAL:HG23	6	0.13
(1,270)	1:63:A:VAL:H	1:65:A:LEU:H	10	0.13
(1,263)	1:63:A:VAL:H	1:115:A:LYS:H	4	0.13
(1,257)	1:60:A:TYR:H	1:62:A:PHE:H	3	0.13
(1,205)	1:51:A:ASP:H	1:55:A:GLN:H	7	0.13
(1,185)	1:49:A:LEU:H	1:52:A:GLU:H	3	0.13
(1,170)	1:49:A:LEU:HD11	1:109:A:LEU:H	5	0.13
(1,170)	1:49:A:LEU:HD12	1:109:A:LEU:H	5	0.13
(1,170)	1:49:A:LEU:HD13	1:109:A:LEU:H	5	0.13
(1,170)	1:49:A:LEU:HD21	1:109:A:LEU:H	5	0.13
(1,170)	1:49:A:LEU:HD22	1:109:A:LEU:H	5	0.13
(1,170)	1:49:A:LEU:HD23	1:109:A:LEU:H	5	0.13
(1,153)	1:47:A:CYS:H	1:52:A:GLU:H	10	0.13
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD11	2	0.13
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD12	2	0.13
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD13	2	0.13
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD11	2	0.13
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD12	2	0.13
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD13	2	0.13
(1,52)	1:32:A:PHE:H	1:135:A:LEU:H	3	0.13
(1,46)	1:31:A:LEU:H	1:65:A:LEU:H	9	0.13
(1,10)	1:26:A:ILE:HD11	1:62:A:PHE:HE1	4	0.13
(1,10)	1:26:A:ILE:HD11	1:62:A:PHE:HE2	4	0.13
(1,10)	1:26:A:ILE:HD12	1:62:A:PHE:HE1	4	0.13
(1,10)	1:26:A:ILE:HD12	1:62:A:PHE:HE2	4	0.13
(1,10)	1:26:A:ILE:HD13	1:62:A:PHE:HE1	4	0.13
(1,10)	1:26:A:ILE:HD13	1:62:A:PHE:HE2	4	0.13
(1,899)	1:222:A:ILE:H	1:222:A:ILE:HD11	9	0.12
(1,899)	1:222:A:ILE:H	1:222:A:ILE:HD12	9	0.12
(1,899)	1:222:A:ILE:H	1:222:A:ILE:HD13	9	0.12
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD11	2	0.12
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD12	2	0.12
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD13	2	0.12
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD21	2	0.12
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD22	2	0.12
(1,880)	1:215:A:GLU:H	1:217:A:LEU:HD23	2	0.12
(1,877)	1:214:A:PHE:HE1	1:218:A:LEU:HD11	4	0.12
(1,877)	1:214:A:PHE:HE1	1:218:A:LEU:HD12	4	0.12
(1,877)	1:214:A:PHE:HE1	1:218:A:LEU:HD13	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:214:A:PHE:HE2	1:218:A:LEU:HD11	4	0.12
(1,877)	1:214:A:PHE:HE2	1:218:A:LEU:HD12	4	0.12
(1,877)	1:214:A:PHE:HE2	1:218:A:LEU:HD13	4	0.12
(1,863)	1:203:A:LEU:H	1:203:A:LEU:HD21	7	0.12
(1,863)	1:203:A:LEU:H	1:203:A:LEU:HD22	7	0.12
(1,863)	1:203:A:LEU:H	1:203:A:LEU:HD23	7	0.12
(1,862)	1:203:A:LEU:H	1:203:A:LEU:HD11	6	0.12
(1,862)	1:203:A:LEU:H	1:203:A:LEU:HD12	6	0.12
(1,862)	1:203:A:LEU:H	1:203:A:LEU:HD13	6	0.12
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD11	8	0.12
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD12	8	0.12
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD13	8	0.12
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD21	8	0.12
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD22	8	0.12
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD23	8	0.12
(1,731)	1:176:A:VAL:HG11	1:183:A:SER:H	4	0.12
(1,731)	1:176:A:VAL:HG12	1:183:A:SER:H	4	0.12
(1,731)	1:176:A:VAL:HG13	1:183:A:SER:H	4	0.12
(1,731)	1:176:A:VAL:HG21	1:183:A:SER:H	4	0.12
(1,731)	1:176:A:VAL:HG22	1:183:A:SER:H	4	0.12
(1,731)	1:176:A:VAL:HG23	1:183:A:SER:H	4	0.12
(1,682)	1:164:A:MET:H	1:165:A:ASP:H	1	0.12
(1,659)	1:159:A:VAL:HG11	1:161:A:ASP:H	6	0.12
(1,659)	1:159:A:VAL:HG12	1:161:A:ASP:H	6	0.12
(1,659)	1:159:A:VAL:HG13	1:161:A:ASP:H	6	0.12
(1,659)	1:159:A:VAL:HG21	1:161:A:ASP:H	6	0.12
(1,659)	1:159:A:VAL:HG22	1:161:A:ASP:H	6	0.12
(1,659)	1:159:A:VAL:HG23	1:161:A:ASP:H	6	0.12
(1,568)	1:145:A:ILE:HD11	1:172:A:ALA:H	4	0.12
(1,568)	1:145:A:ILE:HD12	1:172:A:ALA:H	4	0.12
(1,568)	1:145:A:ILE:HD13	1:172:A:ALA:H	4	0.12
(1,567)	1:145:A:ILE:HD11	1:171:A:ILE:H	5	0.12
(1,567)	1:145:A:ILE:HD12	1:171:A:ILE:H	5	0.12
(1,567)	1:145:A:ILE:HD13	1:171:A:ILE:H	5	0.12
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG11	9	0.12
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG12	9	0.12
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG13	9	0.12
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG21	9	0.12
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG22	9	0.12
(1,542)	1:140:A:ALA:HB1	1:159:A:VAL:HG23	9	0.12
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG11	9	0.12
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG12	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG13	9	0.12
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG21	9	0.12
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG22	9	0.12
(1,542)	1:140:A:ALA:HB2	1:159:A:VAL:HG23	9	0.12
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG11	9	0.12
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG12	9	0.12
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG13	9	0.12
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG21	9	0.12
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG22	9	0.12
(1,542)	1:140:A:ALA:HB3	1:159:A:VAL:HG23	9	0.12
(1,529)	1:139:A:HIS:H	1:140:A:ALA:H	5	0.12
(1,511)	1:136:A:VAL:H	1:156:A:ILE:HD11	6	0.12
(1,511)	1:136:A:VAL:H	1:156:A:ILE:HD12	6	0.12
(1,511)	1:136:A:VAL:H	1:156:A:ILE:HD13	6	0.12
(1,491)	1:135:A:LEU:HD21	1:136:A:VAL:H	4	0.12
(1,491)	1:135:A:LEU:HD22	1:136:A:VAL:H	4	0.12
(1,491)	1:135:A:LEU:HD23	1:136:A:VAL:H	4	0.12
(1,486)	1:134:A:ASP:H	1:135:A:LEU:H	4	0.12
(1,473)	1:129:A:ILE:H	1:133:A:SER:H	6	0.12
(1,380)	1:104:A:ALA:H	1:118:A:GLY:H	10	0.12
(1,379)	1:104:A:ALA:HB1	1:118:A:GLY:H	8	0.12
(1,379)	1:104:A:ALA:HB2	1:118:A:GLY:H	8	0.12
(1,379)	1:104:A:ALA:HB3	1:118:A:GLY:H	8	0.12
(1,348)	1:86:A:GLY:H	1:108:A:VAL:HG11	5	0.12
(1,348)	1:86:A:GLY:H	1:108:A:VAL:HG12	5	0.12
(1,348)	1:86:A:GLY:H	1:108:A:VAL:HG13	5	0.12
(1,348)	1:86:A:GLY:H	1:108:A:VAL:HG21	5	0.12
(1,348)	1:86:A:GLY:H	1:108:A:VAL:HG22	5	0.12
(1,348)	1:86:A:GLY:H	1:108:A:VAL:HG23	5	0.12
(1,295)	1:67:A:ILE:HD11	1:69:A:PHE:HE1	8	0.12
(1,295)	1:67:A:ILE:HD11	1:69:A:PHE:HE2	8	0.12
(1,295)	1:67:A:ILE:HD12	1:69:A:PHE:HE1	8	0.12
(1,295)	1:67:A:ILE:HD12	1:69:A:PHE:HE2	8	0.12
(1,295)	1:67:A:ILE:HD13	1:69:A:PHE:HE1	8	0.12
(1,295)	1:67:A:ILE:HD13	1:69:A:PHE:HE2	8	0.12
(1,262)	1:63:A:VAL:HG11	1:115:A:LYS:H	6	0.12
(1,262)	1:63:A:VAL:HG12	1:115:A:LYS:H	6	0.12
(1,262)	1:63:A:VAL:HG13	1:115:A:LYS:H	6	0.12
(1,262)	1:63:A:VAL:HG21	1:115:A:LYS:H	6	0.12
(1,262)	1:63:A:VAL:HG22	1:115:A:LYS:H	6	0.12
(1,262)	1:63:A:VAL:HG23	1:115:A:LYS:H	6	0.12
(1,257)	1:60:A:TYR:H	1:62:A:PHE:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:49:A:LEU:HD21	1:77:A:PHE:HD1	8	0.12
(1,191)	1:49:A:LEU:HD21	1:77:A:PHE:HD2	8	0.12
(1,191)	1:49:A:LEU:HD22	1:77:A:PHE:HD1	8	0.12
(1,191)	1:49:A:LEU:HD22	1:77:A:PHE:HD2	8	0.12
(1,191)	1:49:A:LEU:HD23	1:77:A:PHE:HD1	8	0.12
(1,191)	1:49:A:LEU:HD23	1:77:A:PHE:HD2	8	0.12
(1,185)	1:49:A:LEU:H	1:52:A:GLU:H	1	0.12
(1,185)	1:49:A:LEU:H	1:52:A:GLU:H	5	0.12
(1,164)	1:48:A:VAL:HG11	1:53:A:PHE:H	8	0.12
(1,164)	1:48:A:VAL:HG12	1:53:A:PHE:H	8	0.12
(1,164)	1:48:A:VAL:HG13	1:53:A:PHE:H	8	0.12
(1,164)	1:48:A:VAL:HG21	1:53:A:PHE:H	8	0.12
(1,164)	1:48:A:VAL:HG22	1:53:A:PHE:H	8	0.12
(1,164)	1:48:A:VAL:HG23	1:53:A:PHE:H	8	0.12
(1,153)	1:47:A:CYS:H	1:52:A:GLU:H	1	0.12
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD11	10	0.12
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD12	10	0.12
(1,112)	1:41:A:PHE:HE1	1:44:A:LEU:HD13	10	0.12
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD11	10	0.12
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD12	10	0.12
(1,112)	1:41:A:PHE:HE2	1:44:A:LEU:HD13	10	0.12
(1,46)	1:31:A:LEU:H	1:65:A:LEU:H	8	0.12
(1,29)	1:31:A:LEU:HD11	1:134:A:ASP:H	3	0.12
(1,29)	1:31:A:LEU:HD12	1:134:A:ASP:H	3	0.12
(1,29)	1:31:A:LEU:HD13	1:134:A:ASP:H	3	0.12
(1,29)	1:31:A:LEU:HD21	1:134:A:ASP:H	3	0.12
(1,29)	1:31:A:LEU:HD22	1:134:A:ASP:H	3	0.12
(1,29)	1:31:A:LEU:HD23	1:134:A:ASP:H	3	0.12
(1,29)	1:31:A:LEU:HD11	1:134:A:ASP:H	8	0.12
(1,29)	1:31:A:LEU:HD12	1:134:A:ASP:H	8	0.12
(1,29)	1:31:A:LEU:HD13	1:134:A:ASP:H	8	0.12
(1,29)	1:31:A:LEU:HD21	1:134:A:ASP:H	8	0.12
(1,29)	1:31:A:LEU:HD22	1:134:A:ASP:H	8	0.12
(1,29)	1:31:A:LEU:HD23	1:134:A:ASP:H	8	0.12
(1,26)	1:30:A:ALA:H	1:32:A:PHE:H	8	0.12
(1,23)	1:30:A:ALA:H	1:135:A:LEU:H	4	0.12
(1,19)	1:30:A:ALA:H	1:133:A:SER:H	4	0.12
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE1	9	0.12
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE2	9	0.12
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE1	9	0.12
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE2	9	0.12
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE1	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE2	9	0.12
(1,4)	1:25:A:ILE:HD11	1:27:A:GLU:H	3	0.12
(1,4)	1:25:A:ILE:HD12	1:27:A:GLU:H	3	0.12
(1,4)	1:25:A:ILE:HD13	1:27:A:GLU:H	3	0.12
(1,890)	1:218:A:LEU:H	1:220:A:GLU:H	5	0.11
(1,859)	1:200:A:THR:H	1:201:A:GLU:H	9	0.11
(1,855)	1:198:A:SER:HB2	1:201:A:GLU:H	4	0.11
(1,855)	1:198:A:SER:HB3	1:201:A:GLU:H	4	0.11
(1,690)	1:170:A:GLN:H	1:173:A:ASP:H	8	0.11
(1,671)	1:159:A:VAL:HB	1:183:A:SER:H	2	0.11
(1,669)	1:159:A:VAL:HG11	1:176:A:VAL:HG11	6	0.11
(1,669)	1:159:A:VAL:HG11	1:176:A:VAL:HG12	6	0.11
(1,669)	1:159:A:VAL:HG11	1:176:A:VAL:HG13	6	0.11
(1,669)	1:159:A:VAL:HG11	1:176:A:VAL:HG21	6	0.11
(1,669)	1:159:A:VAL:HG11	1:176:A:VAL:HG22	6	0.11
(1,669)	1:159:A:VAL:HG11	1:176:A:VAL:HG23	6	0.11
(1,669)	1:159:A:VAL:HG12	1:176:A:VAL:HG11	6	0.11
(1,669)	1:159:A:VAL:HG12	1:176:A:VAL:HG12	6	0.11
(1,669)	1:159:A:VAL:HG12	1:176:A:VAL:HG13	6	0.11
(1,669)	1:159:A:VAL:HG12	1:176:A:VAL:HG21	6	0.11
(1,669)	1:159:A:VAL:HG12	1:176:A:VAL:HG22	6	0.11
(1,669)	1:159:A:VAL:HG12	1:176:A:VAL:HG23	6	0.11
(1,669)	1:159:A:VAL:HG13	1:176:A:VAL:HG11	6	0.11
(1,669)	1:159:A:VAL:HG13	1:176:A:VAL:HG12	6	0.11
(1,669)	1:159:A:VAL:HG13	1:176:A:VAL:HG13	6	0.11
(1,669)	1:159:A:VAL:HG13	1:176:A:VAL:HG21	6	0.11
(1,669)	1:159:A:VAL:HG13	1:176:A:VAL:HG22	6	0.11
(1,669)	1:159:A:VAL:HG13	1:176:A:VAL:HG23	6	0.11
(1,669)	1:159:A:VAL:HG21	1:176:A:VAL:HG11	6	0.11
(1,669)	1:159:A:VAL:HG21	1:176:A:VAL:HG12	6	0.11
(1,669)	1:159:A:VAL:HG21	1:176:A:VAL:HG13	6	0.11
(1,669)	1:159:A:VAL:HG21	1:176:A:VAL:HG21	6	0.11
(1,669)	1:159:A:VAL:HG21	1:176:A:VAL:HG22	6	0.11
(1,669)	1:159:A:VAL:HG21	1:176:A:VAL:HG23	6	0.11
(1,669)	1:159:A:VAL:HG22	1:176:A:VAL:HG11	6	0.11
(1,669)	1:159:A:VAL:HG22	1:176:A:VAL:HG12	6	0.11
(1,669)	1:159:A:VAL:HG22	1:176:A:VAL:HG13	6	0.11
(1,669)	1:159:A:VAL:HG22	1:176:A:VAL:HG21	6	0.11
(1,669)	1:159:A:VAL:HG22	1:176:A:VAL:HG22	6	0.11
(1,669)	1:159:A:VAL:HG22	1:176:A:VAL:HG23	6	0.11
(1,669)	1:159:A:VAL:HG23	1:176:A:VAL:HG11	6	0.11
(1,669)	1:159:A:VAL:HG23	1:176:A:VAL:HG12	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:159:A:VAL:HG23	1:176:A:VAL:HG13	6	0.11
(1,669)	1:159:A:VAL:HG23	1:176:A:VAL:HG21	6	0.11
(1,669)	1:159:A:VAL:HG23	1:176:A:VAL:HG22	6	0.11
(1,669)	1:159:A:VAL:HG23	1:176:A:VAL:HG23	6	0.11
(1,660)	1:159:A:VAL:HG11	1:169:A:GLN:H	10	0.11
(1,660)	1:159:A:VAL:HG12	1:169:A:GLN:H	10	0.11
(1,660)	1:159:A:VAL:HG13	1:169:A:GLN:H	10	0.11
(1,660)	1:159:A:VAL:HG21	1:169:A:GLN:H	10	0.11
(1,660)	1:159:A:VAL:HG22	1:169:A:GLN:H	10	0.11
(1,660)	1:159:A:VAL:HG23	1:169:A:GLN:H	10	0.11
(1,633)	1:156:A:ILE:HD11	1:197:A:ALA:H	10	0.11
(1,633)	1:156:A:ILE:HD12	1:197:A:ALA:H	10	0.11
(1,633)	1:156:A:ILE:HD13	1:197:A:ALA:H	10	0.11
(1,586)	1:148:A:SER:H	1:152:A:ASN:H	4	0.11
(1,577)	1:146:A:LEU:HD11	1:175:A:PHE:HE1	9	0.11
(1,577)	1:146:A:LEU:HD11	1:175:A:PHE:HE2	9	0.11
(1,577)	1:146:A:LEU:HD12	1:175:A:PHE:HE1	9	0.11
(1,577)	1:146:A:LEU:HD12	1:175:A:PHE:HE2	9	0.11
(1,577)	1:146:A:LEU:HD13	1:175:A:PHE:HE1	9	0.11
(1,577)	1:146:A:LEU:HD13	1:175:A:PHE:HE2	9	0.11
(1,577)	1:146:A:LEU:HD21	1:175:A:PHE:HE1	9	0.11
(1,577)	1:146:A:LEU:HD21	1:175:A:PHE:HE2	9	0.11
(1,577)	1:146:A:LEU:HD22	1:175:A:PHE:HE1	9	0.11
(1,577)	1:146:A:LEU:HD22	1:175:A:PHE:HE2	9	0.11
(1,577)	1:146:A:LEU:HD23	1:175:A:PHE:HE1	9	0.11
(1,577)	1:146:A:LEU:HD23	1:175:A:PHE:HE2	9	0.11
(1,521)	1:138:A:SER:H	1:140:A:ALA:H	8	0.11
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD11	9	0.11
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD12	9	0.11
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD13	9	0.11
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD21	9	0.11
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD22	9	0.11
(1,512)	1:136:A:VAL:H	1:195:A:LEU:HD23	9	0.11
(1,495)	1:135:A:LEU:HD11	1:153:A:LYS:H	3	0.11
(1,495)	1:135:A:LEU:HD12	1:153:A:LYS:H	3	0.11
(1,495)	1:135:A:LEU:HD13	1:153:A:LYS:H	3	0.11
(1,495)	1:135:A:LEU:HD21	1:153:A:LYS:H	3	0.11
(1,495)	1:135:A:LEU:HD22	1:153:A:LYS:H	3	0.11
(1,495)	1:135:A:LEU:HD23	1:153:A:LYS:H	3	0.11
(1,494)	1:135:A:LEU:H	1:137:A:ILE:H	7	0.11
(1,482)	1:131:A:ASP:H	1:133:A:SER:H	7	0.11
(1,473)	1:129:A:ILE:H	1:133:A:SER:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD11	9	0.11
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD12	9	0.11
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD13	9	0.11
(1,457)	1:126:A:GLN:H	1:129:A:ILE:H	3	0.11
(1,457)	1:126:A:GLN:H	1:129:A:ILE:H	4	0.11
(1,457)	1:126:A:GLN:H	1:129:A:ILE:H	6	0.11
(1,457)	1:126:A:GLN:H	1:129:A:ILE:H	9	0.11
(1,420)	1:109:A:LEU:HD11	1:114:A:LEU:H	3	0.11
(1,420)	1:109:A:LEU:HD12	1:114:A:LEU:H	3	0.11
(1,420)	1:109:A:LEU:HD13	1:114:A:LEU:H	3	0.11
(1,420)	1:109:A:LEU:HD21	1:114:A:LEU:H	3	0.11
(1,420)	1:109:A:LEU:HD22	1:114:A:LEU:H	3	0.11
(1,420)	1:109:A:LEU:HD23	1:114:A:LEU:H	3	0.11
(1,389)	1:106:A:GLN:H	1:118:A:GLY:H	8	0.11
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD11	7	0.11
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD12	7	0.11
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD13	7	0.11
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD21	7	0.11
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD22	7	0.11
(1,339)	1:82:A:GLN:H	1:109:A:LEU:HD23	7	0.11
(1,310)	1:81:A:VAL:HG11	1:106:A:GLN:H	1	0.11
(1,310)	1:81:A:VAL:HG12	1:106:A:GLN:H	1	0.11
(1,310)	1:81:A:VAL:HG13	1:106:A:GLN:H	1	0.11
(1,310)	1:81:A:VAL:HG21	1:106:A:GLN:H	1	0.11
(1,310)	1:81:A:VAL:HG22	1:106:A:GLN:H	1	0.11
(1,310)	1:81:A:VAL:HG23	1:106:A:GLN:H	1	0.11
(1,308)	1:80:A:LEU:H	1:81:A:VAL:HG21	5	0.11
(1,308)	1:80:A:LEU:H	1:81:A:VAL:HG22	5	0.11
(1,308)	1:80:A:LEU:H	1:81:A:VAL:HG23	5	0.11
(1,273)	1:64:A:ARG:H	1:65:A:LEU:HD11	7	0.11
(1,273)	1:64:A:ARG:H	1:65:A:LEU:HD12	7	0.11
(1,273)	1:64:A:ARG:H	1:65:A:LEU:HD13	7	0.11
(1,273)	1:64:A:ARG:H	1:65:A:LEU:HD21	7	0.11
(1,273)	1:64:A:ARG:H	1:65:A:LEU:HD22	7	0.11
(1,273)	1:64:A:ARG:H	1:65:A:LEU:HD23	7	0.11
(1,257)	1:60:A:TYR:H	1:62:A:PHE:H	6	0.11
(1,231)	1:56:A:GLU:H	1:58:A:ILE:H	10	0.11
(1,205)	1:51:A:ASP:H	1:55:A:GLN:H	6	0.11
(1,204)	1:51:A:ASP:H	1:54:A:CYS:H	3	0.11
(1,185)	1:49:A:LEU:H	1:52:A:GLU:H	4	0.11
(1,185)	1:49:A:LEU:H	1:52:A:GLU:H	9	0.11
(1,169)	1:49:A:LEU:HD21	1:107:A:TYR:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:49:A:LEU:HD22	1:107:A:TYR:H	8	0.11
(1,169)	1:49:A:LEU:HD23	1:107:A:TYR:H	8	0.11
(1,168)	1:49:A:LEU:HD11	1:107:A:TYR:H	2	0.11
(1,168)	1:49:A:LEU:HD12	1:107:A:TYR:H	2	0.11
(1,168)	1:49:A:LEU:HD13	1:107:A:TYR:H	2	0.11
(1,101)	1:39:A:VAL:HG11	1:44:A:LEU:H	1	0.11
(1,101)	1:39:A:VAL:HG12	1:44:A:LEU:H	1	0.11
(1,101)	1:39:A:VAL:HG13	1:44:A:LEU:H	1	0.11
(1,101)	1:39:A:VAL:HG21	1:44:A:LEU:H	1	0.11
(1,101)	1:39:A:VAL:HG22	1:44:A:LEU:H	1	0.11
(1,101)	1:39:A:VAL:HG23	1:44:A:LEU:H	1	0.11
(1,80)	1:33:A:VAL:H	1:68:A:GLN:H	5	0.11
(1,77)	1:33:A:VAL:H	1:66:A:ILE:H	4	0.11
(1,40)	1:31:A:LEU:HD21	1:53:A:PHE:HZ	6	0.11
(1,40)	1:31:A:LEU:HD22	1:53:A:PHE:HZ	6	0.11
(1,40)	1:31:A:LEU:HD23	1:53:A:PHE:HZ	6	0.11
(1,31)	1:31:A:LEU:H	1:135:A:LEU:H	4	0.11
(1,28)	1:30:A:ALA:H	1:64:A:ARG:H	4	0.11
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE1	8	0.11
(1,7)	1:25:A:ILE:HD11	1:62:A:PHE:HE2	8	0.11
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE1	8	0.11
(1,7)	1:25:A:ILE:HD12	1:62:A:PHE:HE2	8	0.11
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE1	8	0.11
(1,7)	1:25:A:ILE:HD13	1:62:A:PHE:HE2	8	0.11
(1,6)	1:25:A:ILE:H	1:27:A:GLU:H	2	0.11
(1,1)	1:25:A:ILE:HD11	1:26:A:ILE:H	9	0.11
(1,1)	1:25:A:ILE:HD12	1:26:A:ILE:H	9	0.11
(1,1)	1:25:A:ILE:HD13	1:26:A:ILE:H	9	0.11
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD11	1	0.1
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD12	1	0.1
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD13	1	0.1
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD21	1	0.1
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD22	1	0.1
(1,773)	1:182:A:TRP:HE1	1:203:A:LEU:HD23	1	0.1
(1,756)	1:181:A:VAL:HG11	1:182:A:TRP:H	9	0.1
(1,756)	1:181:A:VAL:HG12	1:182:A:TRP:H	9	0.1
(1,756)	1:181:A:VAL:HG13	1:182:A:TRP:H	9	0.1
(1,662)	1:159:A:VAL:HG11	1:171:A:ILE:H	7	0.1
(1,662)	1:159:A:VAL:HG12	1:171:A:ILE:H	7	0.1
(1,662)	1:159:A:VAL:HG13	1:171:A:ILE:H	7	0.1
(1,662)	1:159:A:VAL:HG21	1:171:A:ILE:H	7	0.1
(1,662)	1:159:A:VAL:HG22	1:171:A:ILE:H	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:159:A:VAL:HG23	1:171:A:ILE:H	7	0.1
(1,652)	1:157:A:VAL:H	1:184:A:CYS:HG	9	0.1
(1,633)	1:156:A:ILE:HD11	1:197:A:ALA:H	5	0.1
(1,633)	1:156:A:ILE:HD12	1:197:A:ALA:H	5	0.1
(1,633)	1:156:A:ILE:HD13	1:197:A:ALA:H	5	0.1
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG11	3	0.1
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG12	3	0.1
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG13	3	0.1
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG21	3	0.1
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG22	3	0.1
(1,539)	1:140:A:ALA:HB1	1:157:A:VAL:HG23	3	0.1
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG11	3	0.1
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG12	3	0.1
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG13	3	0.1
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG21	3	0.1
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG22	3	0.1
(1,539)	1:140:A:ALA:HB2	1:157:A:VAL:HG23	3	0.1
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG11	3	0.1
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG12	3	0.1
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG13	3	0.1
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG21	3	0.1
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG22	3	0.1
(1,539)	1:140:A:ALA:HB3	1:157:A:VAL:HG23	3	0.1
(1,482)	1:131:A:ASP:H	1:133:A:SER:H	9	0.1
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD11	7	0.1
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD12	7	0.1
(1,460)	1:127:A:SER:H	1:128:A:ILE:HD13	7	0.1
(1,457)	1:126:A:GLN:H	1:129:A:ILE:H	1	0.1
(1,434)	1:114:A:LEU:HD11	1:115:A:LYS:H	5	0.1
(1,434)	1:114:A:LEU:HD12	1:115:A:LYS:H	5	0.1
(1,434)	1:114:A:LEU:HD13	1:115:A:LYS:H	5	0.1
(1,434)	1:114:A:LEU:HD21	1:115:A:LYS:H	5	0.1
(1,434)	1:114:A:LEU:HD22	1:115:A:LYS:H	5	0.1
(1,434)	1:114:A:LEU:HD23	1:115:A:LYS:H	5	0.1
(1,409)	1:108:A:VAL:HG11	1:113:A:LYS:H	7	0.1
(1,409)	1:108:A:VAL:HG12	1:113:A:LYS:H	7	0.1
(1,409)	1:108:A:VAL:HG13	1:113:A:LYS:H	7	0.1
(1,409)	1:108:A:VAL:HG21	1:113:A:LYS:H	7	0.1
(1,409)	1:108:A:VAL:HG22	1:113:A:LYS:H	7	0.1
(1,409)	1:108:A:VAL:HG23	1:113:A:LYS:H	7	0.1
(1,294)	1:67:A:ILE:HD11	1:69:A:PHE:HD1	3	0.1
(1,294)	1:67:A:ILE:HD11	1:69:A:PHE:HD2	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:67:A:ILE:HD12	1:69:A:PHE:HD1	3	0.1
(1,294)	1:67:A:ILE:HD12	1:69:A:PHE:HD2	3	0.1
(1,294)	1:67:A:ILE:HD13	1:69:A:PHE:HD1	3	0.1
(1,294)	1:67:A:ILE:HD13	1:69:A:PHE:HD2	3	0.1
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG11	2	0.1
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG12	2	0.1
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG13	2	0.1
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG21	2	0.1
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG22	2	0.1
(1,276)	1:65:A:LEU:HD11	1:116:A:VAL:HG23	2	0.1
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG11	2	0.1
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG12	2	0.1
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG13	2	0.1
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG21	2	0.1
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG22	2	0.1
(1,276)	1:65:A:LEU:HD12	1:116:A:VAL:HG23	2	0.1
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG11	2	0.1
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG12	2	0.1
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG13	2	0.1
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG21	2	0.1
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG22	2	0.1
(1,276)	1:65:A:LEU:HD13	1:116:A:VAL:HG23	2	0.1
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG11	2	0.1
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG12	2	0.1
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG13	2	0.1
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG21	2	0.1
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG22	2	0.1
(1,276)	1:65:A:LEU:HD21	1:116:A:VAL:HG23	2	0.1
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG11	2	0.1
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG12	2	0.1
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG13	2	0.1
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG21	2	0.1
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG22	2	0.1
(1,276)	1:65:A:LEU:HD22	1:116:A:VAL:HG23	2	0.1
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG11	2	0.1
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG12	2	0.1
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG13	2	0.1
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG21	2	0.1
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG22	2	0.1
(1,276)	1:65:A:LEU:HD23	1:116:A:VAL:HG23	2	0.1
(1,208)	1:52:A:GLU:H	1:55:A:GLN:H	7	0.1
(1,185)	1:49:A:LEU:H	1:52:A:GLU:H	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:49:A:LEU:HD11	1:118:A:GLY:H	10	0.1
(1,180)	1:49:A:LEU:HD12	1:118:A:GLY:H	10	0.1
(1,180)	1:49:A:LEU:HD13	1:118:A:GLY:H	10	0.1
(1,180)	1:49:A:LEU:HD21	1:118:A:GLY:H	10	0.1
(1,180)	1:49:A:LEU:HD22	1:118:A:GLY:H	10	0.1
(1,180)	1:49:A:LEU:HD23	1:118:A:GLY:H	10	0.1
(1,175)	1:49:A:LEU:HD21	1:116:A:VAL:H	10	0.1
(1,175)	1:49:A:LEU:HD22	1:116:A:VAL:H	10	0.1
(1,175)	1:49:A:LEU:HD23	1:116:A:VAL:H	10	0.1
(1,164)	1:48:A:VAL:HG11	1:53:A:PHE:H	2	0.1
(1,164)	1:48:A:VAL:HG12	1:53:A:PHE:H	2	0.1
(1,164)	1:48:A:VAL:HG13	1:53:A:PHE:H	2	0.1
(1,164)	1:48:A:VAL:HG21	1:53:A:PHE:H	2	0.1
(1,164)	1:48:A:VAL:HG22	1:53:A:PHE:H	2	0.1
(1,164)	1:48:A:VAL:HG23	1:53:A:PHE:H	2	0.1
(1,1)	1:25:A:ILE:HD11	1:26:A:ILE:H	2	0.1
(1,1)	1:25:A:ILE:HD12	1:26:A:ILE:H	2	0.1
(1,1)	1:25:A:ILE:HD13	1:26:A:ILE:H	2	0.1

10 Dihedral-angle violation analysis [i](#)

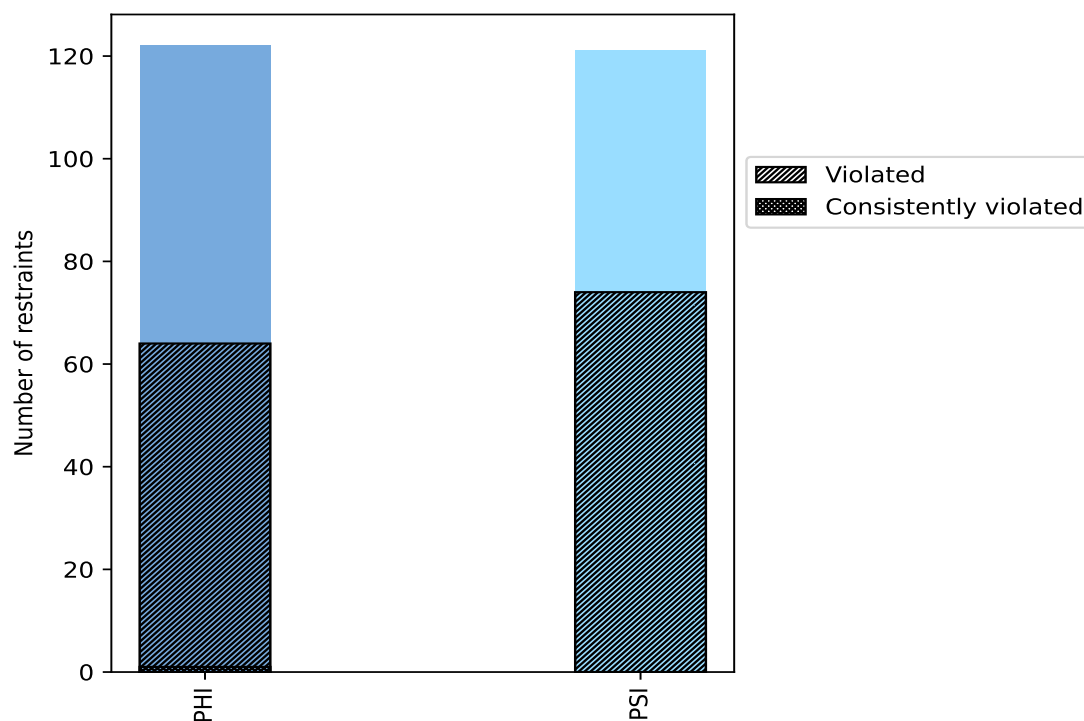
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	122	50.2	64	52.5	26.3	1	0.8	0.4
PSI	121	49.8	74	61.2	30.5	0	0.0	0.0
Total	243	100.0	138	56.8	56.8	1	0.4	0.4

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



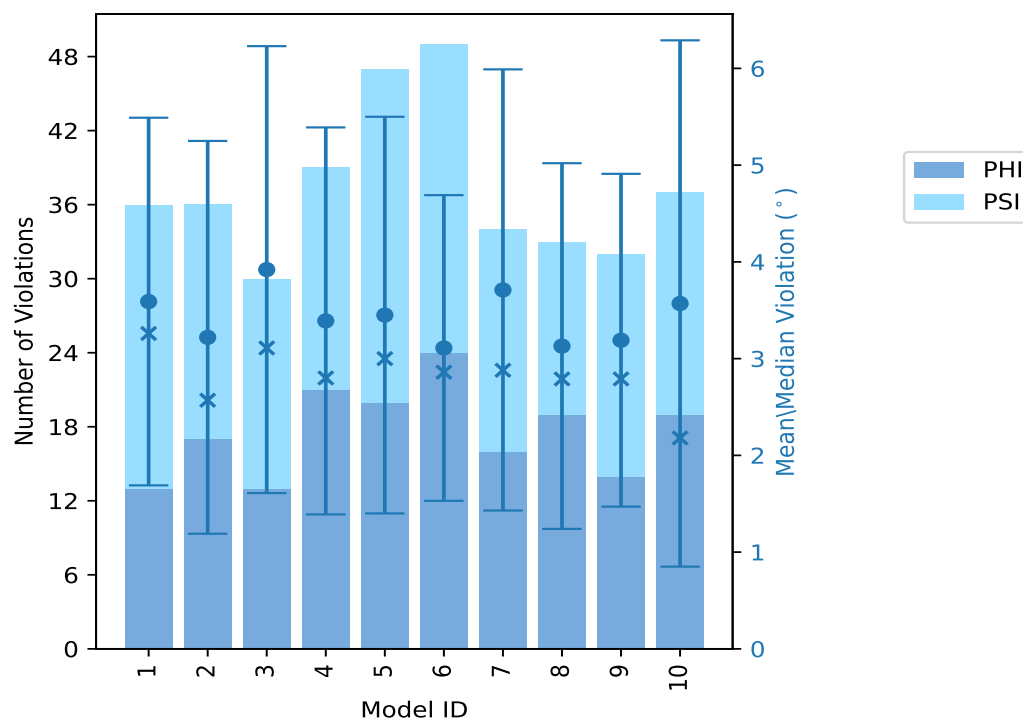
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	13	23	36	3.59	8.93	1.9	3.26
2	17	19	36	3.22	9.03	2.03	2.57
3	13	17	30	3.92	8.96	2.31	3.11
4	21	18	39	3.39	7.89	2.0	2.8
5	20	27	47	3.45	9.32	2.05	3.0
6	24	25	49	3.11	6.98	1.58	2.86
7	16	18	34	3.71	11.43	2.28	2.88
8	19	14	33	3.13	9.04	1.89	2.79
9	14	18	32	3.19	7.67	1.72	2.79
10	19	18	37	3.57	10.26	2.72	2.18

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

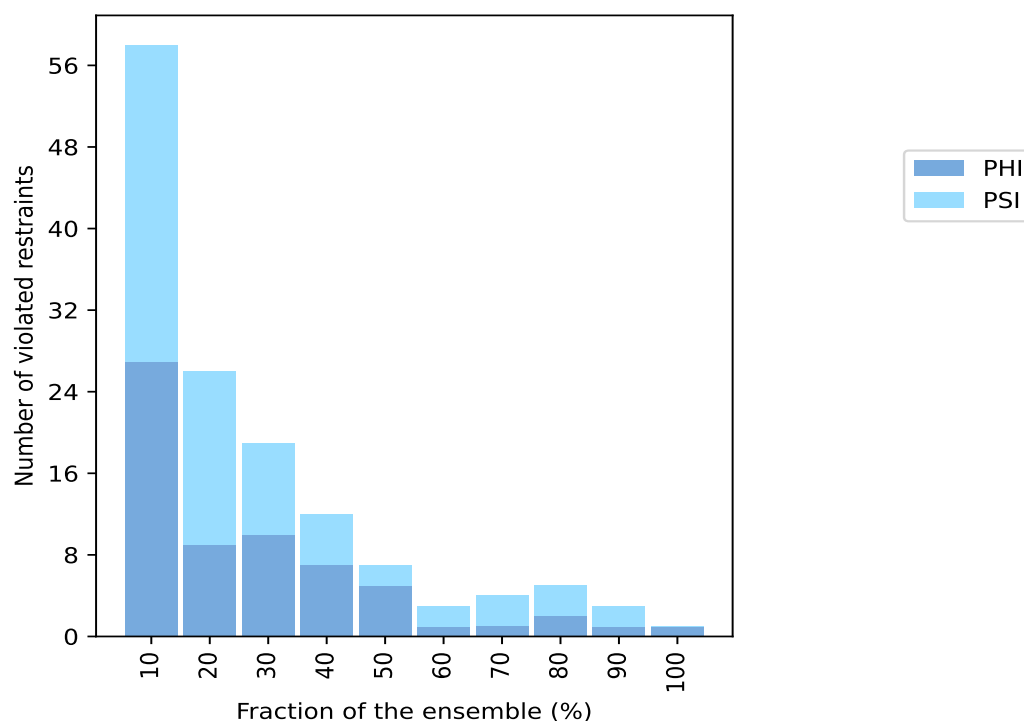
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
27	31	58	1	10.0
9	17	26	2	20.0
10	9	19	3	30.0
7	5	12	4	40.0
5	2	7	5	50.0
1	2	3	6	60.0
1	3	4	7	70.0
2	3	5	8	80.0
1	2	3	9	90.0
1	0	1	10	100.0

¹ Number of models with violations

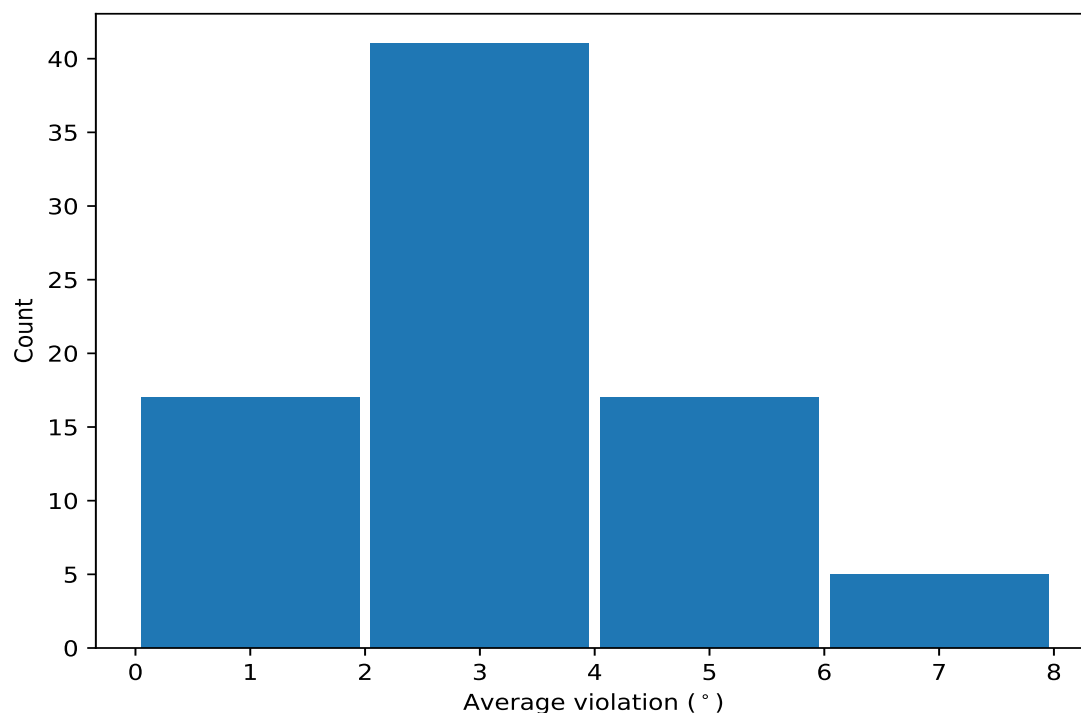
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	10	4.58	2.07	3.68
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	9	3.45	1.35	3.86
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	9	2.81	2.26	2.16
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	9	2.42	1.19	1.93
(1,87)	1:105:A:ARG:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	8	6.19	1.72	5.5
(1,112)	1:126:A:GLN:N	1:126:A:GLN:CA	1:126:A:GLN:C	1:127:A:SER:N	8	4.37	1.62	4.14
(1,160)	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	1:159:A:VAL:N	8	3.64	1.4	3.48
(1,225)	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1:207:A:PRO:N	8	3.51	1.87	3.4
(1,81)	1:97:A:GLN:C	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	8	2.0	0.81	1.54
(1,173)	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	1:173:A:ASP:N	7	5.73	2.43	5.61
(1,169)	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	1:171:A:ILE:N	7	4.29	1.9	4.43
(1,153)	1:154:A:PRO:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	7	3.79	2.44	2.82
(1,138)	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	1:146:A:LEU:N	7	3.0	1.19	2.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,182)	1:176:A:VAL:C	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	6	5.33	2.27	5.21
(1,193)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:GLU:N	6	3.76	2.02	2.92
(1,187)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:CYS:N	6	2.54	1.23	2.12
(1,149)	1:150:A:ARG:C	1:151:A:LEU:N	1:151:A:LEU:CA	1:151:A:LEU:C	5	4.04	1.54	4.3
(1,37)	1:54:A:CYS:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	5	4.03	2.59	2.14
(1,188)	1:183:A:SER:C	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	5	3.6	0.96	3.33
(1,102)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:ILE:N	5	2.97	1.78	2.36
(1,40)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:LEU:N	5	2.7	1.45	2.21
(1,224)	1:205:A:PRO:C	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	5	2.22	0.88	2.06
(1,107)	1:120:A:ASP:C	1:121:A:PHE:N	1:121:A:PHE:CA	1:121:A:PHE:C	5	1.75	0.44	1.84
(1,132)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:HIS:N	4	6.68	1.7	6.68
(1,176)	1:173:A:ASP:C	1:174:A:LYS:N	1:174:A:LYS:CA	1:174:A:LYS:C	4	6.6	3.7	6.0
(1,131)	1:137:A:ILE:C	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	4	6.16	1.69	5.78
(1,76)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	4	5.8	1.09	5.42
(1,101)	1:115:A:LYS:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	4	4.86	1.85	4.44
(1,50)	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	1:62:A:PHE:N	4	4.53	1.66	5.1
(1,113)	1:126:A:GLN:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	4	3.73	2.35	3.12
(1,143)	1:147:A:ASP:C	1:148:A:SER:N	1:148:A:SER:CA	1:148:A:SER:C	4	3.37	1.64	2.92
(1,172)	1:171:A:ILE:C	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	4	3.2	1.77	2.76
(1,82)	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	1:99:A:GLY:N	4	2.92	0.71	2.92
(1,217)	1:199:A:GLN:N	1:199:A:GLN:CA	1:199:A:GLN:C	1:200:A:THR:N	4	2.87	1.73	2.24
(1,11)	1:33:A:VAL:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	4	2.2	0.91	2.15
(1,154)	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	1:156:A:ILE:N	3	5.38	0.75	5.87
(1,168)	1:169:A:GLN:C	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	3	5.21	3.3	4.41
(1,184)	1:177:A:GLU:C	1:178:A:LEU:N	1:178:A:LEU:CA	1:178:A:LEU:C	3	5.08	3.67	2.76
(1,189)	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	1:185:A:ALA:N	3	4.53	2.2	4.56
(1,181)	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	1:177:A:GLU:N	3	4.53	1.48	4.92
(1,145)	1:148:A:SER:C	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	3	3.88	1.16	3.47
(1,14)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:PRO:N	3	3.69	0.67	3.25
(1,80)	1:95:A:ILE:N	1:95:A:ILE:CA	1:95:A:ILE:C	1:96:A:ASP:N	3	3.37	0.76	3.78
(1,48)	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	1:61:A:GLY:N	3	3.31	1.73	3.58
(1,52)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:LEU:N	3	3.17	1.2	3.86
(1,3)	1:29:A:LYS:C	1:30:A:ALA:N	1:30:A:ALA:CA	1:30:A:ALA:C	3	2.98	1.24	2.55
(1,77)	1:92:A:LYS:C	1:93:A:ILE:N	1:93:A:ILE:CA	1:93:A:ILE:C	3	2.63	1.85	1.42
(1,35)	1:53:A:PHE:C	1:54:A:CYS:N	1:54:A:CYS:CA	1:54:A:CYS:C	3	2.63	0.72	2.23
(1,84)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:CYS:N	3	2.2	0.65	1.97
(1,171)	1:171:A:ILE:N	1:171:A:ILE:CA	1:171:A:ILE:C	1:172:A:ALA:N	3	1.97	0.45	1.73
(1,55)	1:65:A:LEU:C	1:66:A:ILE:N	1:66:A:ILE:CA	1:66:A:ILE:C	3	1.91	1.0	1.31
(1,9)	1:32:A:PHE:C	1:33:A:VAL:N	1:33:A:VAL:CA	1:33:A:VAL:C	3	1.82	0.24	1.7
(1,49)	1:60:A:TYR:C	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	3	1.82	0.48	1.71
(1,95)	1:111:A:ASN:C	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	3	1.32	0.22	1.26
(1,98)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:LYS:N	2	6.23	3.09	6.23
(1,78)	1:93:A:ILE:N	1:93:A:ILE:CA	1:93:A:ILE:C	1:94:A:PRO:N	2	5.19	0.38	5.19
(1,134)	1:143:A:GLY:N	1:143:A:GLY:CA	1:143:A:GLY:C	1:144:A:SER:N	2	4.34	3.16	4.34
(1,135)	1:143:A:GLY:C	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	2	3.72	0.82	3.72
(1,1)	1:28:A:GLU:C	1:29:A:LYS:N	1:29:A:LYS:CA	1:29:A:LYS:C	2	3.45	1.28	3.45
(1,117)	1:128:A:ILE:C	1:129:A:ILE:N	1:129:A:ILE:CA	1:129:A:ILE:C	2	3.38	1.51	3.38
(1,175)	1:173:A:ASP:N	1:173:A:ASP:CA	1:173:A:ASP:C	1:174:A:LYS:N	2	3.28	0.47	3.28
(1,209)	1:195:A:LEU:N	1:195:A:LEU:CA	1:195:A:LEU:C	1:196:A:ARG:N	2	2.74	0.11	2.74
(1,36)	1:54:A:CYS:N	1:54:A:CYS:CA	1:54:A:CYS:C	1:55:A:GLN:N	2	2.59	1.11	2.59
(1,130)	1:137:A:ILE:N	1:137:A:ILE:CA	1:137:A:ILE:C	1:138:A:SER:N	2	2.58	0.07	2.58

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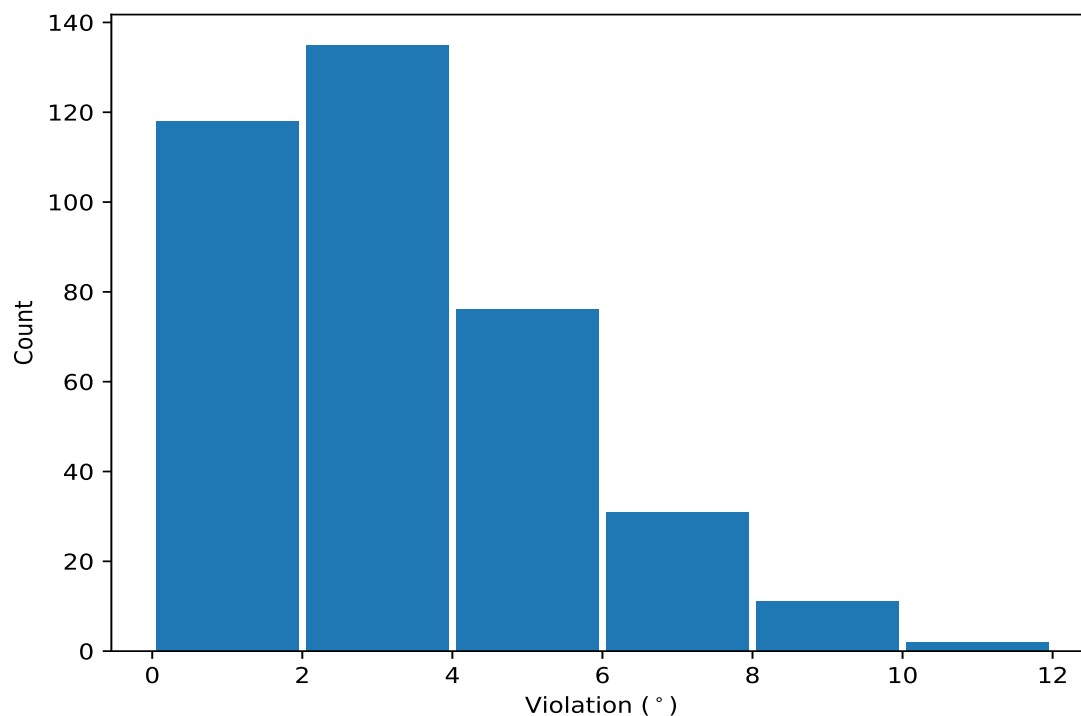
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,31)	1:51:A:ASP:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	2	2.38	1.36	2.38
(1,32)	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1:53:A:PHE:N	2	2.32	0.09	2.32
(1,6)	1:31:A:LEU:N	1:31:A:LEU:CA	1:31:A:LEU:C	1:32:A:PHE:N	2	2.13	0.86	2.13
(1,15)	1:40:A:PRO:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	2	2.12	0.69	2.12
(1,106)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:PHE:N	2	2.04	0.76	2.04
(1,229)	1:214:A:PHE:N	1:214:A:PHE:CA	1:214:A:PHE:C	1:215:A:GLU:N	2	1.92	0.48	1.92
(1,207)	1:194:A:GLY:N	1:194:A:GLY:CA	1:194:A:GLY:C	1:195:A:LEU:N	2	1.86	0.13	1.86
(1,186)	1:182:A:TRP:C	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	2	1.83	0.13	1.83
(1,180)	1:175:A:PHE:C	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	2	1.81	0.34	1.81
(1,79)	1:94:A:PRO:C	1:95:A:ILE:N	1:95:A:ILE:CA	1:95:A:ILE:C	2	1.68	0.33	1.68
(1,62)	1:73:A:TYR:N	1:73:A:TYR:CA	1:73:A:TYR:C	1:74:A:SER:N	2	1.56	0.47	1.56
(1,30)	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	1:52:A:GLU:N	2	1.48	0.33	1.48
(1,179)	1:175:A:PHE:N	1:175:A:PHE:CA	1:175:A:PHE:C	1:176:A:VAL:N	2	1.35	0.14	1.35
(1,142)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:SER:N	2	1.33	0.22	1.33
(1,144)	1:148:A:SER:N	1:148:A:SER:CA	1:148:A:SER:C	1:149:A:LEU:N	2	1.3	0.08	1.3
(1,29)	1:50:A:SER:C	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	2	1.22	0.05	1.22

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [\(i\)](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,176)	1:173:A:ASP:C	1:174:A:LYS:N	1:174:A:LYS:CA	1:174:A:LYS:C	7	11.43
(1,184)	1:177:A:GLU:C	1:178:A:LEU:N	1:178:A:LEU:CA	1:178:A:LEU:C	10	10.26
(1,87)	1:105:A:ARG:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	10	9.69
(1,168)	1:169:A:GLN:C	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	10	9.59
(1,98)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:LYS:N	5	9.32
(1,173)	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	1:173:A:ASP:N	8	9.04
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	2	9.03
(1,176)	1:173:A:ASP:C	1:174:A:LYS:N	1:174:A:LYS:CA	1:174:A:LYS:C	3	8.96
(1,182)	1:176:A:VAL:C	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	1	8.93
(1,131)	1:137:A:ILE:C	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	10	8.79
(1,132)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:HIS:N	10	8.62
(1,173)	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	1:173:A:ASP:N	3	8.15
(1,132)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:HIS:N	3	8.12
(1,164)	1:167:A:HIS:C	1:168:A:GLN:N	1:168:A:GLN:CA	1:168:A:GLN:C	4	7.89
(1,37)	1:54:A:CYS:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	5	7.83
(1,87)	1:105:A:ARG:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	3	7.79
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	10	7.79
(1,153)	1:154:A:PRO:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	4	7.78
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	9	7.67
(1,101)	1:115:A:LYS:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	5	7.62
(1,76)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	1	7.54
(1,173)	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	1:173:A:ASP:N	7	7.52
(1,134)	1:143:A:GLY:N	1:143:A:GLY:CA	1:143:A:GLY:C	1:144:A:SER:N	7	7.49
(1,112)	1:126:A:GLN:N	1:126:A:GLN:CA	1:126:A:GLN:C	1:127:A:SER:N	3	7.45
(1,100)	1:115:A:LYS:N	1:115:A:LYS:CA	1:115:A:LYS:C	1:116:A:VAL:N	2	7.27
(1,189)	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	1:185:A:ALA:N	4	7.21
(1,113)	1:126:A:GLN:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	7	7.15
(1,193)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:GLU:N	4	7.05
(1,87)	1:105:A:ARG:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	6	6.98
(1,182)	1:176:A:VAL:C	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	5	6.91
(1,122)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:TYR:N	4	6.86
(1,169)	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	1:171:A:ILE:N	3	6.67
(1,37)	1:54:A:CYS:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	4	6.47
(1,182)	1:176:A:VAL:C	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	9	6.45
(1,160)	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	1:159:A:VAL:N	1	6.43
(1,131)	1:137:A:ILE:C	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	5	6.4
(1,133)	1:142:A:THR:C	1:143:A:GLY:N	1:143:A:GLY:CA	1:143:A:GLY:C	6	6.25
(1,225)	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1:207:A:PRO:N	1	6.22
(1,169)	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	1:171:A:ILE:N	8	6.16
(1,225)	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1:207:A:PRO:N	7	6.13
(1,181)	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	1:177:A:GLU:N	9	6.11
(1,50)	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	1:62:A:PHE:N	2	6.08
(1,112)	1:126:A:GLN:N	1:126:A:GLN:CA	1:126:A:GLN:C	1:127:A:SER:N	5	6.04
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	2	6.02
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	7	5.99
(1,172)	1:171:A:ILE:C	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	6	5.95
(1,154)	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	1:156:A:ILE:N	4	5.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,149)	1:150:A:ARG:C	1:151:A:LEU:N	1:151:A:LEU:CA	1:151:A:LEU:C	8	5.93
(1,153)	1:154:A:PRO:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	3	5.92
(1,193)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:GLU:N	7	5.91
(1,76)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	8	5.9
(1,154)	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	1:156:A:ILE:N	1	5.87
(1,87)	1:105:A:ARG:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	2	5.83
(1,143)	1:147:A:ASP:C	1:148:A:SER:N	1:148:A:SER:CA	1:148:A:SER:C	8	5.81
(1,217)	1:199:A:GLN:N	1:199:A:GLN:CA	1:199:A:GLN:C	1:200:A:THR:N	2	5.72
(1,50)	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	1:62:A:PHE:N	1	5.68
(1,153)	1:154:A:PRO:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	6	5.65
(1,173)	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	1:173:A:ASP:N	2	5.61
(1,78)	1:93:A:ILE:N	1:93:A:ILE:CA	1:93:A:ILE:C	1:94:A:PRO:N	7	5.57
(1,102)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:ILE:N	5	5.55
(1,169)	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	1:171:A:ILE:N	6	5.47
(1,145)	1:148:A:SER:C	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	5	5.46
(1,166)	1:168:A:GLN:C	1:169:A:GLN:N	1:169:A:GLN:CA	1:169:A:GLN:C	9	5.45
(1,101)	1:115:A:LYS:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1	5.44
(1,48)	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	1:61:A:GLY:N	10	5.28
(1,77)	1:92:A:LYS:C	1:93:A:ILE:N	1:93:A:ILE:CA	1:93:A:ILE:C	5	5.25
(1,163)	1:167:A:HIS:N	1:167:A:HIS:CA	1:167:A:HIS:C	1:168:A:GLN:N	4	5.23
(1,132)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:HIS:N	5	5.23
(1,116)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:C	1:129:A:ILE:N	6	5.18
(1,87)	1:105:A:ARG:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	8	5.18
(1,131)	1:137:A:ILE:C	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	3	5.15
(1,188)	1:183:A:SER:C	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	6	5.1
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	1	5.09
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	3	5.09
(1,40)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:LEU:N	8	5.06
(1,74)	1:87:A:GLN:N	1:87:A:GLN:CA	1:87:A:GLN:C	1:88:A:ARG:N	6	5.04
(1,108)	1:121:A:PHE:N	1:121:A:PHE:CA	1:121:A:PHE:C	1:122:A:SER:N	1	5.01
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	6	4.99
(1,87)	1:105:A:ARG:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	9	4.95
(1,87)	1:105:A:ARG:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	4	4.94
(1,76)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	10	4.93
(1,181)	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	1:177:A:GLU:N	10	4.92
(1,46)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:TYR:N	5	4.9
(1,117)	1:128:A:ILE:C	1:129:A:ILE:N	1:129:A:ILE:CA	1:129:A:ILE:C	2	4.89
(1,78)	1:93:A:ILE:N	1:93:A:ILE:CA	1:93:A:ILE:C	1:94:A:PRO:N	1	4.81
(1,76)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	9	4.81
(1,132)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:HIS:N	7	4.76
(1,149)	1:150:A:ARG:C	1:151:A:LEU:N	1:151:A:LEU:CA	1:151:A:LEU:C	4	4.74
(1,1)	1:28:A:GLU:C	1:29:A:LYS:N	1:29:A:LYS:CA	1:29:A:LYS:C	6	4.73
(1,187)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:CYS:N	9	4.67
(1,3)	1:29:A:LYS:C	1:30:A:ALA:N	1:30:A:ALA:CA	1:30:A:ALA:C	10	4.67
(1,113)	1:126:A:GLN:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	5	4.66
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	6	4.65
(1,14)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:PRO:N	3	4.64
(1,138)	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	1:146:A:LEU:N	2	4.63
(1,173)	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	1:173:A:ASP:N	10	4.58
(1,189)	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	1:185:A:ALA:N	9	4.56
(1,102)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:ILE:N	8	4.55

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,135)	1:143:A:GLY:C	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	6	4.54
(1,45)	1:58:A:ILE:C	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	5	4.54
(1,160)	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	1:159:A:VAL:N	2	4.53
(1,112)	1:126:A:GLN:N	1:126:A:GLN:CA	1:126:A:GLN:C	1:127:A:SER:N	6	4.53
(1,50)	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	1:62:A:PHE:N	8	4.52
(1,160)	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	1:159:A:VAL:N	9	4.5
(1,174)	1:172:A:ALA:C	1:173:A:ASP:N	1:173:A:ASP:CA	1:173:A:ASP:C	1	4.48
(1,169)	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	1:171:A:ILE:N	7	4.43
(1,168)	1:169:A:GLN:C	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	1	4.41
(1,54)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:ILE:N	5	4.33
(1,225)	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1:207:A:PRO:N	5	4.31
(1,154)	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	1:156:A:ILE:N	5	4.31
(1,149)	1:150:A:ARG:C	1:151:A:LEU:N	1:151:A:LEU:CA	1:151:A:LEU:C	6	4.3
(1,131)	1:137:A:ILE:C	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	7	4.29
(1,112)	1:126:A:GLN:N	1:126:A:GLN:CA	1:126:A:GLN:C	1:127:A:SER:N	2	4.28
(1,188)	1:183:A:SER:C	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	9	4.26
(1,138)	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	1:146:A:LEU:N	5	4.25
(1,225)	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1:207:A:PRO:N	3	4.2
(1,87)	1:105:A:ARG:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	7	4.17
(1,52)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:LEU:N	2	4.16
(1,241)	1:220:A:GLU:N	1:220:A:GLU:CA	1:220:A:GLU:C	1:221:A:THR:N	6	4.06
(1,80)	1:95:A:ILE:N	1:95:A:ILE:CA	1:95:A:ILE:C	1:96:A:ASP:N	4	4.02
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	2	3.99
(1,169)	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	1:171:A:ILE:N	5	3.99
(1,112)	1:126:A:GLN:N	1:126:A:GLN:CA	1:126:A:GLN:C	1:127:A:SER:N	8	3.99
(1,182)	1:176:A:VAL:C	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	10	3.97
(1,149)	1:150:A:ARG:C	1:151:A:LEU:N	1:151:A:LEU:CA	1:151:A:LEU:C	10	3.96
(1,82)	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	1:99:A:GLY:N	9	3.93
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	5	3.93
(1,143)	1:147:A:ASP:C	1:148:A:SER:N	1:148:A:SER:CA	1:148:A:SER:C	5	3.92
(1,138)	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	1:146:A:LEU:N	7	3.91
(1,112)	1:126:A:GLN:N	1:126:A:GLN:CA	1:126:A:GLN:C	1:127:A:SER:N	1	3.87
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	7	3.86
(1,52)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:LEU:N	1	3.86
(1,224)	1:205:A:PRO:C	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	5	3.81
(1,80)	1:95:A:ILE:N	1:95:A:ILE:CA	1:95:A:ILE:C	1:96:A:ASP:N	1	3.78
(1,175)	1:173:A:ASP:N	1:173:A:ASP:CA	1:173:A:ASP:C	1:174:A:LYS:N	1	3.76
(1,31)	1:51:A:ASP:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	6	3.73
(1,36)	1:54:A:CYS:N	1:54:A:CYS:CA	1:54:A:CYS:C	1:55:A:GLN:N	4	3.7
(1,187)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:CYS:N	3	3.65
(1,35)	1:53:A:PHE:C	1:54:A:CYS:N	1:54:A:CYS:CA	1:54:A:CYS:C	4	3.64
(1,170)	1:170:A:GLN:C	1:171:A:ILE:N	1:171:A:ILE:CA	1:171:A:ILE:C	6	3.63
(1,160)	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	1:159:A:VAL:N	7	3.6
(1,22)	1:45:A:VAL:N	1:45:A:VAL:CA	1:45:A:VAL:C	1:46:A:SER:N	9	3.59
(1,48)	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	1:61:A:GLY:N	3	3.58
(1,41)	1:56:A:GLU:C	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	5	3.55
(1,40)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:LEU:N	9	3.55
(1,172)	1:171:A:ILE:C	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	4	3.51
(1,193)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:GLU:N	2	3.5
(1,58)	1:67:A:ILE:N	1:67:A:ILE:CA	1:67:A:ILE:C	1:68:A:GLN:N	6	3.5
(1,11)	1:33:A:VAL:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	2	3.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,145)	1:148:A:SER:C	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	4	3.47
(1,101)	1:115:A:LYS:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	4	3.44
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	3	3.43
(1,160)	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	1:159:A:VAL:N	6	3.35
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	8	3.35
(1,188)	1:183:A:SER:C	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	1	3.33
(1,13)	1:38:A:THR:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	8	3.32
(1,55)	1:65:A:LEU:C	1:66:A:ILE:N	1:66:A:ILE:CA	1:66:A:ILE:C	2	3.31
(1,81)	1:97:A:GLN:C	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	6	3.29
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	4	3.29
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	4	3.26
(1,81)	1:97:A:GLN:C	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	1	3.26
(1,185)	1:178:A:LEU:N	1:178:A:LEU:CA	1:178:A:LEU:C	1:179:A:GLY:N	1	3.25
(1,14)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:PRO:N	9	3.25
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	1	3.19
(1,14)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:PRO:N	5	3.19
(1,98)	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1:115:A:LYS:N	3	3.14
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	3	3.08
(1,84)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:CYS:N	7	3.08
(1,103)	1:116:A:VAL:C	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	6	3.06
(1,182)	1:176:A:VAL:C	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	2	3.04
(1,176)	1:173:A:ASP:C	1:174:A:LYS:N	1:174:A:LYS:CA	1:174:A:LYS:C	8	3.04
(1,82)	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	1:99:A:GLY:N	10	3.04
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	8	3.0
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	5	3.0
(1,16)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:PRO:N	9	3.0
(1,6)	1:31:A:LEU:N	1:31:A:LEU:CA	1:31:A:LEU:C	1:32:A:PHE:N	10	3.0
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	4	2.98
(1,176)	1:173:A:ASP:C	1:174:A:LYS:N	1:174:A:LYS:CA	1:174:A:LYS:C	6	2.96
(1,101)	1:115:A:LYS:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	8	2.95
(1,223)	1:204:A:LYS:N	1:204:A:LYS:CA	1:204:A:LYS:C	1:205:A:PRO:N	6	2.92
(1,112)	1:126:A:GLN:N	1:126:A:GLN:CA	1:126:A:GLN:C	1:127:A:SER:N	7	2.92
(1,135)	1:143:A:GLY:C	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1	2.91
(1,159)	1:157:A:VAL:C	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	6	2.89
(1,173)	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	1:173:A:ASP:N	1	2.88
(1,195)	1:188:A:GLU:N	1:188:A:GLU:CA	1:188:A:GLU:C	1:189:A:THR:N	6	2.86
(1,209)	1:195:A:LEU:N	1:195:A:LEU:CA	1:195:A:LEU:C	1:196:A:ARG:N	1	2.85
(1,127)	1:135:A:LEU:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	7	2.85
(1,153)	1:154:A:PRO:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	9	2.82
(1,175)	1:173:A:ASP:N	1:173:A:ASP:CA	1:173:A:ASP:C	1:174:A:LYS:N	10	2.81
(1,15)	1:40:A:PRO:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	7	2.81
(1,217)	1:199:A:GLN:N	1:199:A:GLN:CA	1:199:A:GLN:C	1:200:A:THR:N	8	2.8
(1,138)	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	1:146:A:LEU:N	6	2.8
(1,106)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:PHE:N	4	2.8
(1,82)	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	1:99:A:GLY:N	3	2.8
(1,28)	1:48:A:VAL:N	1:48:A:VAL:CA	1:48:A:VAL:C	1:49:A:LEU:N	8	2.79
(1,184)	1:177:A:GLU:C	1:178:A:LEU:N	1:178:A:LEU:CA	1:178:A:LEU:C	9	2.76
(1,24)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:CYS:N	5	2.74
(1,188)	1:183:A:SER:C	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	4	2.71
(1,145)	1:148:A:SER:C	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	3	2.7
(1,182)	1:176:A:VAL:C	1:177:A:GLU:N	1:177:A:GLU:CA	1:177:A:GLU:C	3	2.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,160)	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	1:159:A:VAL:N	10	2.65
(1,130)	1:137:A:ILE:N	1:137:A:ILE:CA	1:137:A:ILE:C	1:138:A:SER:N	4	2.65
(1,209)	1:195:A:LEU:N	1:195:A:LEU:CA	1:195:A:LEU:C	1:196:A:ARG:N	2	2.63
(1,225)	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1:207:A:PRO:N	9	2.6
(1,171)	1:171:A:ILE:N	1:171:A:ILE:CA	1:171:A:ILE:C	1:172:A:ALA:N	1	2.6
(1,188)	1:183:A:SER:C	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	3	2.58
(1,181)	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	1:177:A:GLU:N	6	2.55
(1,3)	1:29:A:LYS:C	1:30:A:ALA:N	1:30:A:ALA:CA	1:30:A:ALA:C	5	2.55
(1,91)	1:107:A:TYR:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	6	2.54
(1,11)	1:33:A:VAL:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	9	2.52
(1,231)	1:215:A:GLU:N	1:215:A:GLU:CA	1:215:A:GLU:C	1:216:A:ARG:N	7	2.51
(1,60)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:TYR:N	2	2.51
(1,130)	1:137:A:ILE:N	1:137:A:ILE:CA	1:137:A:ILE:C	1:138:A:SER:N	1	2.5
(1,49)	1:60:A:TYR:C	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	5	2.46
(1,23)	1:45:A:VAL:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	6	2.46
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	3	2.43
(1,64)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:VAL:N	5	2.41
(1,32)	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1:53:A:PHE:N	5	2.41
(1,229)	1:214:A:PHE:N	1:214:A:PHE:CA	1:214:A:PHE:C	1:215:A:GLU:N	7	2.4
(1,81)	1:97:A:GLN:C	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	9	2.38
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	7	2.38
(1,102)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:ILE:N	3	2.36
(1,187)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:CYS:N	7	2.35
(1,146)	1:149:A:LEU:N	1:149:A:LEU:CA	1:149:A:LEU:C	1:150:A:ARG:N	6	2.34
(1,193)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:GLU:N	3	2.33
(1,80)	1:95:A:ILE:N	1:95:A:ILE:CA	1:95:A:ILE:C	1:96:A:ASP:N	5	2.31
(1,173)	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	1:173:A:ASP:N	5	2.3
(1,138)	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	1:146:A:LEU:N	9	2.26
(1,92)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:LEU:N	6	2.26
(1,2)	1:29:A:LYS:N	1:29:A:LYS:CA	1:29:A:LYS:C	1:30:A:ALA:N	3	2.26
(1,107)	1:120:A:ASP:C	1:121:A:PHE:N	1:121:A:PHE:CA	1:121:A:PHE:C	4	2.25
(1,212)	1:196:A:ARG:C	1:197:A:ALA:N	1:197:A:ALA:CA	1:197:A:ALA:C	2	2.23
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	8	2.23
(1,184)	1:177:A:GLU:C	1:178:A:LEU:N	1:178:A:LEU:CA	1:178:A:LEU:C	7	2.23
(1,35)	1:53:A:PHE:C	1:54:A:CYS:N	1:54:A:CYS:CA	1:54:A:CYS:C	6	2.23
(1,32)	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1:53:A:PHE:N	4	2.22
(1,40)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:LEU:N	10	2.21
(1,169)	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	1:171:A:ILE:N	9	2.2
(1,160)	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	1:159:A:VAL:N	4	2.19
(1,75)	1:87:A:GLN:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	10	2.18
(1,1)	1:28:A:GLU:C	1:29:A:LYS:N	1:29:A:LYS:CA	1:29:A:LYS:C	1	2.17
(1,107)	1:120:A:ASP:C	1:121:A:PHE:N	1:121:A:PHE:CA	1:121:A:PHE:C	8	2.16
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	9	2.16
(1,9)	1:32:A:PHE:C	1:33:A:VAL:N	1:33:A:VAL:CA	1:33:A:VAL:C	4	2.15
(1,180)	1:175:A:PHE:C	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	10	2.14
(1,37)	1:54:A:CYS:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	8	2.14
(1,224)	1:205:A:PRO:C	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1	2.12
(1,37)	1:54:A:CYS:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	2	2.07
(1,224)	1:205:A:PRO:C	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	6	2.06
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	10	2.04
(1,62)	1:73:A:TYR:N	1:73:A:TYR:CA	1:73:A:TYR:C	1:74:A:SER:N	2	2.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,224)	1:205:A:PRO:C	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	7	2.02
(1,172)	1:171:A:ILE:C	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	10	2.01
(1,79)	1:94:A:PRO:C	1:95:A:ILE:N	1:95:A:ILE:CA	1:95:A:ILE:C	7	2.01
(1,35)	1:53:A:PHE:C	1:54:A:CYS:N	1:54:A:CYS:CA	1:54:A:CYS:C	7	2.01
(1,207)	1:194:A:GLY:N	1:194:A:GLY:CA	1:194:A:GLY:C	1:195:A:LEU:N	4	1.99
(1,84)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:CYS:N	6	1.97
(1,186)	1:182:A:TRP:C	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	10	1.96
(1,104)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	1:118:A:GLY:N	5	1.96
(1,193)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:GLU:N	8	1.95
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	2	1.93
(1,138)	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	1:146:A:LEU:N	1	1.93
(1,82)	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	1:99:A:GLY:N	5	1.93
(1,143)	1:147:A:ASP:C	1:148:A:SER:N	1:148:A:SER:CA	1:148:A:SER:C	4	1.92
(1,187)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:CYS:N	1	1.9
(1,112)	1:126:A:GLN:N	1:126:A:GLN:CA	1:126:A:GLN:C	1:127:A:SER:N	10	1.9
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	6	1.9
(1,153)	1:154:A:PRO:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	7	1.88
(1,160)	1:158:A:CYS:N	1:158:A:CYS:CA	1:158:A:CYS:C	1:159:A:VAL:N	8	1.87
(1,117)	1:128:A:ILE:C	1:129:A:ILE:N	1:129:A:ILE:CA	1:129:A:ILE:C	6	1.87
(1,225)	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1:207:A:PRO:N	10	1.84
(1,193)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:GLU:N	10	1.84
(1,107)	1:120:A:ASP:C	1:121:A:PHE:N	1:121:A:PHE:CA	1:121:A:PHE:C	10	1.84
(1,189)	1:184:A:CYS:N	1:184:A:CYS:CA	1:184:A:CYS:C	1:185:A:ALA:N	3	1.83
(1,50)	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	1:62:A:PHE:N	6	1.83
(1,162)	1:166:A:ASN:C	1:167:A:HIS:N	1:167:A:HIS:CA	1:167:A:HIS:C	8	1.82
(1,143)	1:147:A:ASP:C	1:148:A:SER:N	1:148:A:SER:CA	1:148:A:SER:C	7	1.82
(1,30)	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	1:52:A:GLU:N	5	1.81
(1,11)	1:33:A:VAL:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	4	1.78
(1,207)	1:194:A:GLY:N	1:194:A:GLY:CA	1:194:A:GLY:C	1:195:A:LEU:N	10	1.73
(1,171)	1:171:A:ILE:N	1:171:A:ILE:CA	1:171:A:ILE:C	1:172:A:ALA:N	5	1.73
(1,202)	1:191:A:LEU:C	1:192:A:ILE:N	1:192:A:ILE:CA	1:192:A:ILE:C	4	1.72
(1,3)	1:29:A:LYS:C	1:30:A:ALA:N	1:30:A:ALA:CA	1:30:A:ALA:C	8	1.72
(1,49)	1:60:A:TYR:C	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	9	1.71
(1,186)	1:182:A:TRP:C	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	8	1.7
(1,9)	1:32:A:PHE:C	1:33:A:VAL:N	1:33:A:VAL:CA	1:33:A:VAL:C	8	1.7
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	4	1.68
(1,217)	1:199:A:GLN:N	1:199:A:GLN:CA	1:199:A:GLN:C	1:200:A:THR:N	6	1.67
(1,37)	1:54:A:CYS:C	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	6	1.66
(1,168)	1:169:A:GLN:C	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	2	1.63
(1,81)	1:97:A:GLN:C	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	5	1.63
(1,95)	1:111:A:ASN:C	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	1	1.61
(1,40)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:LEU:N	3	1.61
(1,9)	1:32:A:PHE:C	1:33:A:VAL:N	1:33:A:VAL:CA	1:33:A:VAL:C	5	1.61
(1,171)	1:171:A:ILE:N	1:171:A:ILE:CA	1:171:A:ILE:C	1:172:A:ALA:N	2	1.59
(1,225)	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1:207:A:PRO:N	4	1.57
(1,113)	1:126:A:GLN:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	10	1.57
(1,142)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:SER:N	2	1.55
(1,84)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:CYS:N	4	1.55
(1,113)	1:126:A:GLN:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	2	1.54
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1	1.5
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	9	1.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,179)	1:175:A:PHE:N	1:175:A:PHE:CA	1:175:A:PHE:C	1:176:A:VAL:N	7	1.49
(1,52)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:LEU:N	6	1.48
(1,36)	1:54:A:CYS:N	1:54:A:CYS:CA	1:54:A:CYS:C	1:55:A:GLN:N	1	1.48
(1,216)	1:198:A:SER:C	1:199:A:GLN:N	1:199:A:GLN:CA	1:199:A:GLN:C	2	1.47
(1,187)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:CYS:N	6	1.47
(1,180)	1:175:A:PHE:C	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	6	1.47
(1,229)	1:214:A:PHE:N	1:214:A:PHE:CA	1:214:A:PHE:C	1:215:A:GLU:N	6	1.44
(1,153)	1:154:A:PRO:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	10	1.44
(1,81)	1:97:A:GLN:C	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	8	1.44
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	8	1.44
(1,18)	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	1:44:A:LEU:N	10	1.44
(1,15)	1:40:A:PRO:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	2	1.43
(1,77)	1:92:A:LYS:C	1:93:A:ILE:N	1:93:A:ILE:CA	1:93:A:ILE:C	3	1.42
(1,167)	1:169:A:GLN:N	1:169:A:GLN:CA	1:169:A:GLN:C	1:170:A:GLN:N	5	1.41
(1,81)	1:97:A:GLN:C	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	4	1.4
(1,165)	1:168:A:GLN:N	1:168:A:GLN:CA	1:168:A:GLN:C	1:169:A:GLN:N	5	1.39
(1,194)	1:187:A:THR:C	1:188:A:GLU:N	1:188:A:GLU:CA	1:188:A:GLU:C	10	1.38
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	10	1.38
(1,144)	1:148:A:SER:N	1:148:A:SER:CA	1:148:A:SER:C	1:149:A:LEU:N	10	1.38
(1,107)	1:120:A:ASP:C	1:121:A:PHE:N	1:121:A:PHE:CA	1:121:A:PHE:C	9	1.38
(1,102)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:ILE:N	7	1.37
(1,81)	1:97:A:GLN:C	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	7	1.36
(1,79)	1:94:A:PRO:C	1:95:A:ILE:N	1:95:A:ILE:CA	1:95:A:ILE:C	4	1.35
(1,172)	1:171:A:ILE:C	1:172:A:ALA:N	1:172:A:ALA:CA	1:172:A:ALA:C	9	1.34
(1,51)	1:63:A:VAL:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	3	1.33
(1,55)	1:65:A:LEU:C	1:66:A:ILE:N	1:66:A:ILE:CA	1:66:A:ILE:C	7	1.31
(1,217)	1:199:A:GLN:N	1:199:A:GLN:CA	1:199:A:GLN:C	1:200:A:THR:N	9	1.3
(1,152)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:PRO:N	5	1.3
(1,49)	1:60:A:TYR:C	1:61:A:GLY:N	1:61:A:GLY:CA	1:61:A:GLY:C	2	1.29
(1,106)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:PHE:N	1	1.28
(1,141)	1:146:A:LEU:C	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	8	1.27
(1,29)	1:50:A:SER:C	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	4	1.27
(1,6)	1:31:A:LEU:N	1:31:A:LEU:CA	1:31:A:LEU:C	1:32:A:PHE:N	5	1.27
(1,95)	1:111:A:ASN:C	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	8	1.26
(1,149)	1:150:A:ARG:C	1:151:A:LEU:N	1:151:A:LEU:CA	1:151:A:LEU:C	7	1.25
(1,138)	1:145:A:ILE:N	1:145:A:ILE:CA	1:145:A:ILE:C	1:146:A:LEU:N	4	1.25
(1,187)	1:183:A:SER:N	1:183:A:SER:CA	1:183:A:SER:C	1:184:A:CYS:N	4	1.23
(1,81)	1:97:A:GLN:C	1:98:A:PHE:N	1:98:A:PHE:CA	1:98:A:PHE:C	2	1.23
(1,72)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:GLY:N	10	1.23
(1,144)	1:148:A:SER:N	1:148:A:SER:CA	1:148:A:SER:C	1:149:A:LEU:N	5	1.22
(1,77)	1:92:A:LYS:C	1:93:A:ILE:N	1:93:A:ILE:CA	1:93:A:ILE:C	4	1.22
(1,179)	1:175:A:PHE:N	1:175:A:PHE:CA	1:175:A:PHE:C	1:176:A:VAL:N	9	1.21
(1,225)	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	1:207:A:PRO:N	6	1.19
(1,134)	1:143:A:GLY:N	1:143:A:GLY:CA	1:143:A:GLY:C	1:144:A:SER:N	6	1.18
(1,29)	1:50:A:SER:C	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	8	1.17
(1,17)	1:42:A:PRO:C	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	5	1.17
(1,30)	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	1:52:A:GLU:N	1	1.15
(1,191)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:PRO:N	9	1.14
(1,107)	1:120:A:ASP:C	1:121:A:PHE:N	1:121:A:PHE:CA	1:121:A:PHE:C	3	1.11
(1,25)	1:46:A:SER:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	6	1.11
(1,224)	1:205:A:PRO:C	1:206:A:PHE:N	1:206:A:PHE:CA	1:206:A:PHE:C	2	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,190)	1:184:A:CYS:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	5	1.1
(1,142)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:SER:N	6	1.1
(1,123)	1:131:A:ASP:C	1:132:A:TYR:N	1:132:A:TYR:CA	1:132:A:TYR:C	10	1.1
(1,55)	1:65:A:LEU:C	1:66:A:ILE:N	1:66:A:ILE:CA	1:66:A:ILE:C	1	1.1
(1,203)	1:192:A:ILE:N	1:192:A:ILE:CA	1:192:A:ILE:C	1:193:A:ALA:N	1	1.09
(1,169)	1:170:A:GLN:N	1:170:A:GLN:CA	1:170:A:GLN:C	1:171:A:ILE:N	2	1.09
(1,139)	1:145:A:ILE:C	1:146:A:LEU:N	1:146:A:LEU:CA	1:146:A:LEU:C	9	1.09
(1,95)	1:111:A:ASN:C	1:112:A:GLY:N	1:112:A:GLY:CA	1:112:A:GLY:C	2	1.09
(1,62)	1:73:A:TYR:N	1:73:A:TYR:CA	1:73:A:TYR:C	1:74:A:SER:N	5	1.09
(1,34)	1:53:A:PHE:N	1:53:A:PHE:CA	1:53:A:PHE:C	1:54:A:CYS:N	2	1.09
(1,48)	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	1:61:A:GLY:N	8	1.06
(1,44)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:GLN:N	6	1.05
(1,40)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:LEU:N	2	1.05
(1,102)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:ILE:N	9	1.04
(1,69)	1:82:A:GLN:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	10	1.04
(1,153)	1:154:A:PRO:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	8	1.03
(1,31)	1:51:A:ASP:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	3	1.02
(1,232)	1:215:A:GLU:C	1:216:A:ARG:N	1:216:A:ARG:CA	1:216:A:ARG:C	6	1.01
(1,11)	1:33:A:VAL:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	5	1.01
(1,33)	1:52:A:GLU:C	1:53:A:PHE:N	1:53:A:PHE:CA	1:53:A:PHE:C	5	1.0